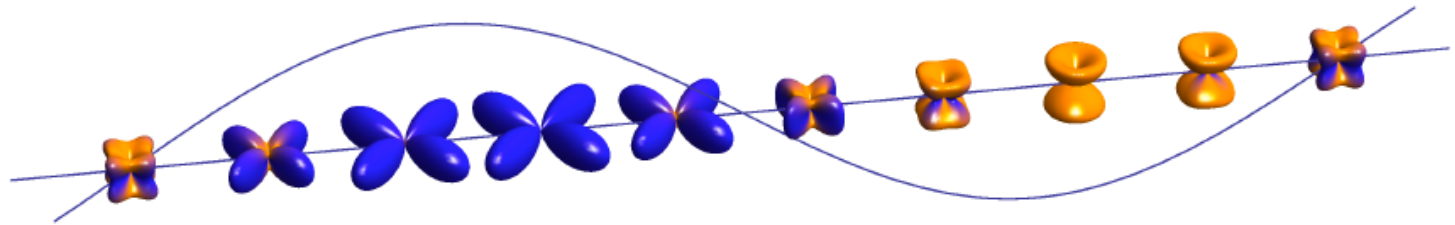
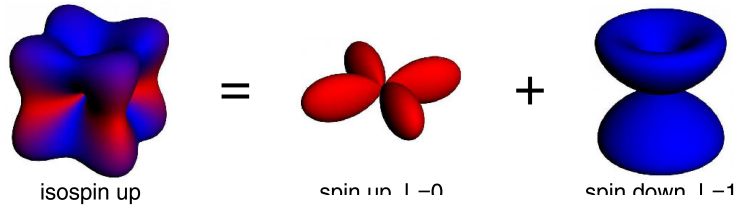


# Resonant X-ray Scattering: Application to Iridates

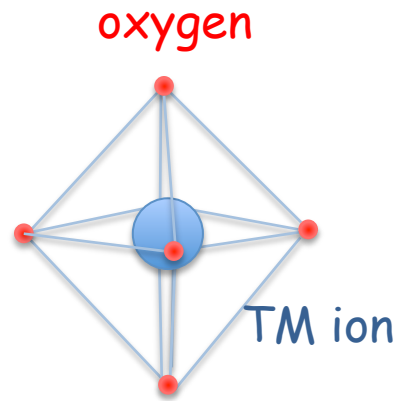
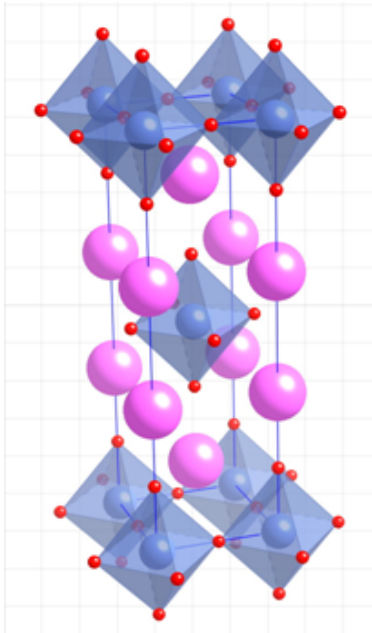


B. J. Kim

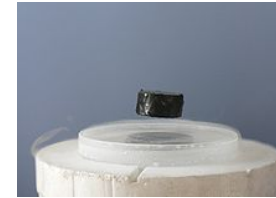
Max Planck Institute for Solid State Research

# Transition metal oxides: Diverse Properties

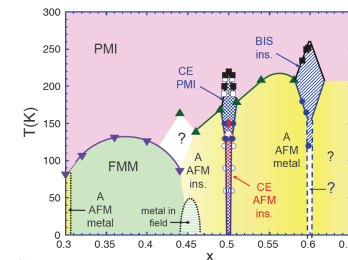
(Layered) Perovskite structure



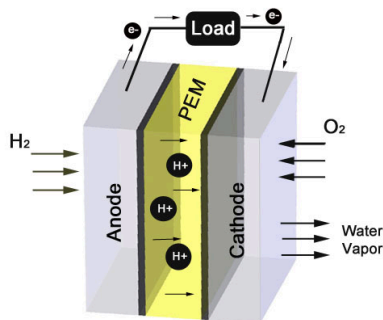
**Cu:** high- $T_c$  superconductivity



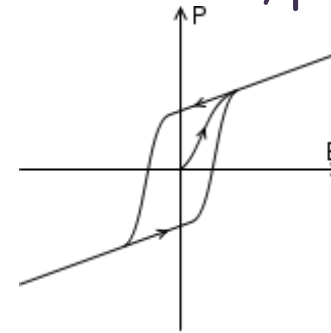
**Mn:** Colossal magnetoresistance



**Ni:** Fuel cell cathodes

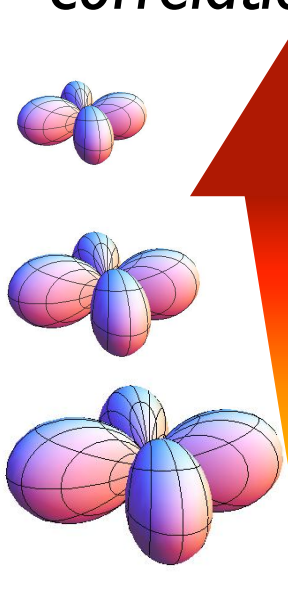


**Ti:** ferroelectric, piezoelectric



# Transition metal oxides

*Strong electron correlation*

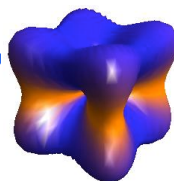
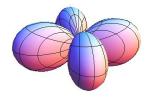


|    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|
| Sc | Ti | V  | Cr | Mn | Fe | Co | Ni | Cu | Zn |
| Y  | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd |
| Lu | Hf | Ta | W  | Re | Os | Ir | Pt | Au | Hg |

3d

4d

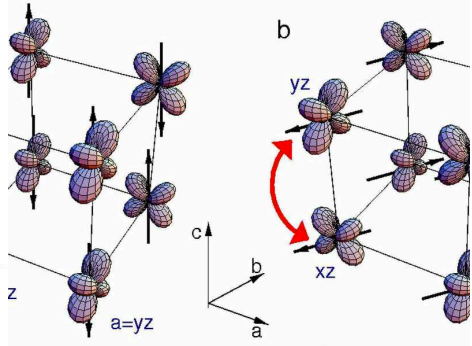
5d



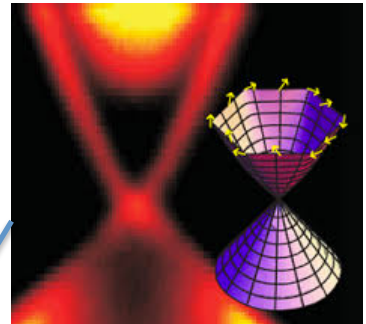
$U \sim 2 \text{ eV}$   
 $\xi_{SO} \sim 0.5 \text{ eV}$

*Strong spin-orbit coupling*

# Correlation + Spin-Orbit Coupling



- high Tc superconductivity
- colossal magnetoresistance



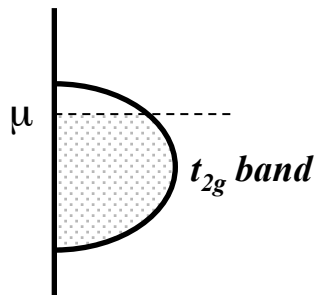
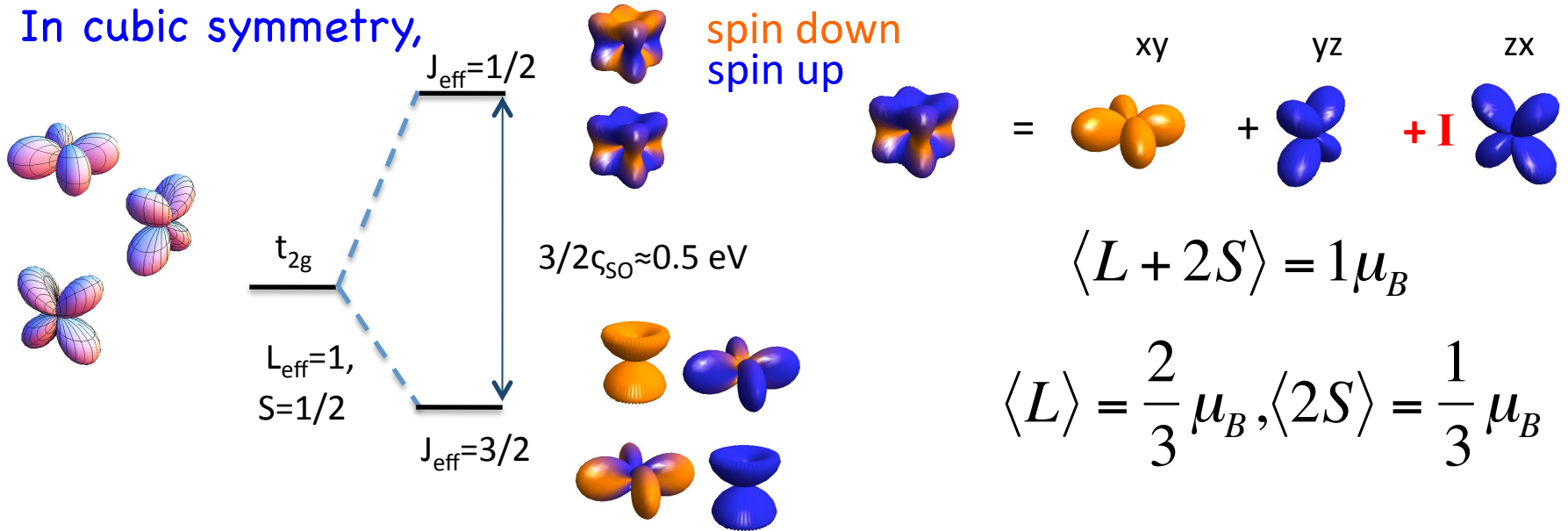
- topological insulator

- novel topological phases
- Kitaev quantum spin liquid
- unconventional superconductivity

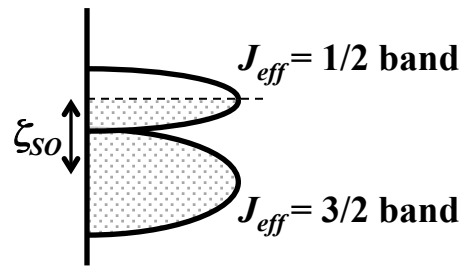
|  |   |   |   |   |   |   |   |    |    |    |                            |                           |                            |                           |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|--|---|---|---|---|---|---|---|----|----|----|----------------------------|---------------------------|----------------------------|---------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
|  | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13                         | 14                        | 15                         | 16                        | 17                       | 18                       |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | boron<br>5<br>10.811       | carbon<br>6<br>12.011     | nitrogen<br>7<br>14.007    | oxygen<br>8<br>15.999     | fluorine<br>9<br>18.998  | helium<br>2<br>4.0026    |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | aluminum<br>13<br>26.982   | silicon<br>14<br>28.086   | phosphorus<br>15<br>30.974 | sulfur<br>16<br>32.065    | chlorine<br>17<br>35.45  | neon<br>10<br>20.180     |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | gallium<br>31<br>69.723    | germanium<br>32<br>72.61  | arsenic<br>33<br>74.922    | selenium<br>34<br>78.96   | bromine<br>35<br>79.904  | argon<br>18<br>39.948    |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | indium<br>49<br>114.82     | tin<br>50<br>118.71       | antimony<br>51<br>121.76   | tellurium<br>52<br>127.60 | iodine<br>53<br>126.90   | krypton<br>36<br>83.80   |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | thallium<br>81<br>204.38   | lead<br>82<br>207.2       | bismuth<br>83<br>208.98    | polonium<br>84<br>[209]   | astatine<br>85<br>[210]  | xenon<br>54<br>131.29    |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unquadrium<br>114<br>[289] | unpentium<br>115<br>[288] | unhexium<br>116<br>[292]   | unseptium<br>117<br>[291] | unoctium<br>118<br>[294] | cesium<br>55<br>132.91   |                          |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unseptium<br>111<br>[272]  | unnilium<br>112<br>[277]  | unnilium<br>113<br>[284]   | unnilium<br>114<br>[289]  | unnilium<br>115<br>[288] | unnilium<br>116<br>[292] | unnilium<br>117<br>[291] |                          |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>110<br>[271]   | unnilium<br>111<br>[272]  | unnilium<br>112<br>[277]   | unnilium<br>113<br>[284]  | unnilium<br>114<br>[289] | unnilium<br>115<br>[288] | unnilium<br>116<br>[292] | unnilium<br>117<br>[291] |                          |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>109<br>[268]   | unnilium<br>110<br>[271]  | unnilium<br>111<br>[272]   | unnilium<br>112<br>[277]  | unnilium<br>113<br>[284] | unnilium<br>114<br>[289] | unnilium<br>115<br>[288] | unnilium<br>116<br>[292] | unnilium<br>117<br>[291] |                          |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>108<br>[269]   | unnilium<br>109<br>[268]  | unnilium<br>110<br>[271]   | unnilium<br>111<br>[272]  | unnilium<br>112<br>[277] | unnilium<br>113<br>[284] | unnilium<br>114<br>[289] | unnilium<br>115<br>[288] | unnilium<br>116<br>[292] | unnilium<br>117<br>[291] |                          |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>107<br>[264]   | unnilium<br>108<br>[269]  | unnilium<br>109<br>[268]   | unnilium<br>110<br>[271]  | unnilium<br>111<br>[272] | unnilium<br>112<br>[277] | unnilium<br>113<br>[284] | unnilium<br>114<br>[289] | unnilium<br>115<br>[288] | unnilium<br>116<br>[292] | unnilium<br>117<br>[291] |                          |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>106<br>[266]   | unnilium<br>107<br>[264]  | unnilium<br>108<br>[269]   | unnilium<br>109<br>[268]  | unnilium<br>110<br>[271] | unnilium<br>111<br>[272] | unnilium<br>112<br>[277] | unnilium<br>113<br>[284] | unnilium<br>114<br>[289] | unnilium<br>115<br>[288] | unnilium<br>116<br>[292] | unnilium<br>117<br>[291] |                          |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>105<br>[262]   | unnilium<br>106<br>[261]  | unnilium<br>107<br>[262]   | unnilium<br>108<br>[266]  | unnilium<br>109<br>[269] | unnilium<br>110<br>[264] | unnilium<br>111<br>[269] | unnilium<br>112<br>[268] | unnilium<br>113<br>[271] | unnilium<br>114<br>[276] | unnilium<br>115<br>[275] | unnilium<br>116<br>[279] | unnilium<br>117<br>[274] |                          |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>104<br>[261]   | unnilium<br>105<br>[262]  | unnilium<br>106<br>[266]   | unnilium<br>107<br>[269]  | unnilium<br>108<br>[264] | unnilium<br>109<br>[269] | unnilium<br>110<br>[268] | unnilium<br>111<br>[271] | unnilium<br>112<br>[276] | unnilium<br>113<br>[275] | unnilium<br>114<br>[279] | unnilium<br>115<br>[274] | unnilium<br>116<br>[278] | unnilium<br>117<br>[273] |                          |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>103<br>[262]   | unnilium<br>104<br>[261]  | unnilium<br>105<br>[262]   | unnilium<br>106<br>[266]  | unnilium<br>107<br>[269] | unnilium<br>108<br>[264] | unnilium<br>109<br>[269] | unnilium<br>110<br>[268] | unnilium<br>111<br>[271] | unnilium<br>112<br>[276] | unnilium<br>113<br>[275] | unnilium<br>114<br>[279] | unnilium<br>115<br>[274] | unnilium<br>116<br>[278] | unnilium<br>117<br>[273] |                          |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>102<br>[262]   | unnilium<br>103<br>[261]  | unnilium<br>104<br>[262]   | unnilium<br>105<br>[266]  | unnilium<br>106<br>[269] | unnilium<br>107<br>[264] | unnilium<br>108<br>[269] | unnilium<br>109<br>[268] | unnilium<br>110<br>[271] | unnilium<br>111<br>[276] | unnilium<br>112<br>[275] | unnilium<br>113<br>[279] | unnilium<br>114<br>[274] | unnilium<br>115<br>[278] | unnilium<br>116<br>[273] | unnilium<br>117<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>101<br>[262]   | unnilium<br>102<br>[261]  | unnilium<br>103<br>[262]   | unnilium<br>104<br>[266]  | unnilium<br>105<br>[269] | unnilium<br>106<br>[264] | unnilium<br>107<br>[269] | unnilium<br>108<br>[268] | unnilium<br>109<br>[271] | unnilium<br>110<br>[276] | unnilium<br>111<br>[275] | unnilium<br>112<br>[279] | unnilium<br>113<br>[274] | unnilium<br>114<br>[278] | unnilium<br>115<br>[273] | unnilium<br>116<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>100<br>[262]   | unnilium<br>101<br>[261]  | unnilium<br>102<br>[262]   | unnilium<br>103<br>[266]  | unnilium<br>104<br>[269] | unnilium<br>105<br>[264] | unnilium<br>106<br>[269] | unnilium<br>107<br>[268] | unnilium<br>108<br>[271] | unnilium<br>109<br>[276] | unnilium<br>110<br>[275] | unnilium<br>111<br>[279] | unnilium<br>112<br>[274] | unnilium<br>113<br>[278] | unnilium<br>114<br>[273] | unnilium<br>115<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>99<br>[262]    | unnilium<br>100<br>[261]  | unnilium<br>101<br>[262]   | unnilium<br>102<br>[266]  | unnilium<br>103<br>[269] | unnilium<br>104<br>[264] | unnilium<br>105<br>[269] | unnilium<br>106<br>[268] | unnilium<br>107<br>[271] | unnilium<br>108<br>[276] | unnilium<br>109<br>[275] | unnilium<br>110<br>[279] | unnilium<br>111<br>[274] | unnilium<br>112<br>[278] | unnilium<br>113<br>[273] | unnilium<br>114<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>98<br>[262]    | unnilium<br>99<br>[261]   | unnilium<br>100<br>[262]   | unnilium<br>101<br>[266]  | unnilium<br>102<br>[269] | unnilium<br>103<br>[264] | unnilium<br>104<br>[269] | unnilium<br>105<br>[268] | unnilium<br>106<br>[271] | unnilium<br>107<br>[276] | unnilium<br>108<br>[275] | unnilium<br>109<br>[279] | unnilium<br>110<br>[274] | unnilium<br>111<br>[278] | unnilium<br>112<br>[273] | unnilium<br>113<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>97<br>[262]    | unnilium<br>98<br>[261]   | unnilium<br>99<br>[262]    | unnilium<br>100<br>[266]  | unnilium<br>101<br>[269] | unnilium<br>102<br>[264] | unnilium<br>103<br>[269] | unnilium<br>104<br>[268] | unnilium<br>105<br>[271] | unnilium<br>106<br>[276] | unnilium<br>107<br>[275] | unnilium<br>108<br>[279] | unnilium<br>109<br>[274] | unnilium<br>110<br>[278] | unnilium<br>111<br>[273] | unnilium<br>112<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>96<br>[262]    | unnilium<br>97<br>[261]   | unnilium<br>98<br>[262]    | unnilium<br>99<br>[266]   | unnilium<br>100<br>[269] | unnilium<br>101<br>[264] | unnilium<br>102<br>[269] | unnilium<br>103<br>[268] | unnilium<br>104<br>[271] | unnilium<br>105<br>[276] | unnilium<br>106<br>[275] | unnilium<br>107<br>[279] | unnilium<br>108<br>[274] | unnilium<br>109<br>[278] | unnilium<br>110<br>[273] | unnilium<br>111<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>95<br>[262]    | unnilium<br>96<br>[261]   | unnilium<br>97<br>[262]    | unnilium<br>98<br>[266]   | unnilium<br>99<br>[269]  | unnilium<br>100<br>[264] | unnilium<br>101<br>[269] | unnilium<br>102<br>[268] | unnilium<br>103<br>[271] | unnilium<br>104<br>[276] | unnilium<br>105<br>[275] | unnilium<br>106<br>[279] | unnilium<br>107<br>[274] | unnilium<br>108<br>[278] | unnilium<br>109<br>[273] | unnilium<br>110<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>94<br>[262]    | unnilium<br>95<br>[261]   | unnilium<br>96<br>[262]    | unnilium<br>97<br>[266]   | unnilium<br>98<br>[269]  | unnilium<br>99<br>[264]  | unnilium<br>100<br>[269] | unnilium<br>101<br>[268] | unnilium<br>102<br>[271] | unnilium<br>103<br>[276] | unnilium<br>104<br>[275] | unnilium<br>105<br>[279] | unnilium<br>106<br>[274] | unnilium<br>107<br>[278] | unnilium<br>108<br>[273] | unnilium<br>109<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>93<br>[262]    | unnilium<br>94<br>[261]   | unnilium<br>95<br>[262]    | unnilium<br>96<br>[266]   | unnilium<br>97<br>[269]  | unnilium<br>98<br>[264]  | unnilium<br>99<br>[269]  | unnilium<br>100<br>[268] | unnilium<br>101<br>[271] | unnilium<br>102<br>[276] | unnilium<br>103<br>[275] | unnilium<br>104<br>[279] | unnilium<br>105<br>[274] | unnilium<br>106<br>[278] | unnilium<br>107<br>[273] | unnilium<br>108<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>92<br>[262]    | unnilium<br>93<br>[261]   | unnilium<br>94<br>[262]    | unnilium<br>95<br>[266]   | unnilium<br>96<br>[269]  | unnilium<br>97<br>[264]  | unnilium<br>98<br>[269]  | unnilium<br>99<br>[268]  | unnilium<br>100<br>[271] | unnilium<br>101<br>[276] | unnilium<br>102<br>[275] | unnilium<br>103<br>[279] | unnilium<br>104<br>[274] | unnilium<br>105<br>[278] | unnilium<br>106<br>[273] | unnilium<br>107<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>91<br>[262]    | unnilium<br>92<br>[261]   | unnilium<br>93<br>[262]    | unnilium<br>94<br>[266]   | unnilium<br>95<br>[269]  | unnilium<br>96<br>[264]  | unnilium<br>97<br>[269]  | unnilium<br>98<br>[268]  | unnilium<br>99<br>[271]  | unnilium<br>100<br>[276] | unnilium<br>101<br>[275] | unnilium<br>102<br>[279] | unnilium<br>103<br>[274] | unnilium<br>104<br>[278] | unnilium<br>105<br>[273] | unnilium<br>106<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>90<br>[262]    | unnilium<br>91<br>[261]   | unnilium<br>92<br>[262]    | unnilium<br>93<br>[266]   | unnilium<br>94<br>[269]  | unnilium<br>95<br>[264]  | unnilium<br>96<br>[269]  | unnilium<br>97<br>[268]  | unnilium<br>98<br>[271]  | unnilium<br>99<br>[276]  | unnilium<br>100<br>[275] | unnilium<br>101<br>[279] | unnilium<br>102<br>[274] | unnilium<br>103<br>[278] | unnilium<br>104<br>[273] | unnilium<br>105<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>89<br>[262]    | unnilium<br>90<br>[261]   | unnilium<br>91<br>[262]    | unnilium<br>92<br>[266]   | unnilium<br>93<br>[269]  | unnilium<br>94<br>[264]  | unnilium<br>95<br>[269]  | unnilium<br>96<br>[268]  | unnilium<br>97<br>[271]  | unnilium<br>98<br>[276]  | unnilium<br>99<br>[275]  | unnilium<br>100<br>[279] | unnilium<br>101<br>[274] | unnilium<br>102<br>[278] | unnilium<br>103<br>[273] | unnilium<br>104<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>88<br>[262]    | unnilium<br>89<br>[261]   | unnilium<br>90<br>[262]    | unnilium<br>91<br>[266]   | unnilium<br>92<br>[269]  | unnilium<br>93<br>[264]  | unnilium<br>94<br>[269]  | unnilium<br>95<br>[268]  | unnilium<br>96<br>[271]  | unnilium<br>97<br>[276]  | unnilium<br>98<br>[275]  | unnilium<br>99<br>[279]  | unnilium<br>100<br>[274] | unnilium<br>101<br>[278] | unnilium<br>102<br>[273] | unnilium<br>103<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>87<br>[262]    | unnilium<br>88<br>[261]   | unnilium<br>89<br>[262]    | unnilium<br>90<br>[266]   | unnilium<br>91<br>[269]  | unnilium<br>92<br>[264]  | unnilium<br>93<br>[269]  | unnilium<br>94<br>[268]  | unnilium<br>95<br>[271]  | unnilium<br>96<br>[276]  | unnilium<br>97<br>[275]  | unnilium<br>98<br>[279]  | unnilium<br>99<br>[274]  | unnilium<br>100<br>[278] | unnilium<br>101<br>[273] | unnilium<br>102<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>86<br>[262]    | unnilium<br>87<br>[261]   | unnilium<br>88<br>[262]    | unnilium<br>89<br>[266]   | unnilium<br>90<br>[269]  | unnilium<br>91<br>[264]  | unnilium<br>92<br>[269]  | unnilium<br>93<br>[268]  | unnilium<br>94<br>[271]  | unnilium<br>95<br>[276]  | unnilium<br>96<br>[275]  | unnilium<br>97<br>[279]  | unnilium<br>98<br>[274]  | unnilium<br>99<br>[278]  | unnilium<br>100<br>[273] | unnilium<br>101<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>85<br>[262]    | unnilium<br>86<br>[261]   | unnilium<br>87<br>[262]    | unnilium<br>88<br>[266]   | unnilium<br>89<br>[269]  | unnilium<br>90<br>[264]  | unnilium<br>91<br>[269]  | unnilium<br>92<br>[268]  | unnilium<br>93<br>[271]  | unnilium<br>94<br>[276]  | unnilium<br>95<br>[275]  | unnilium<br>96<br>[279]  | unnilium<br>97<br>[274]  | unnilium<br>98<br>[278]  | unnilium<br>99<br>[273]  | unnilium<br>100<br>[277] |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>84<br>[262]    | unnilium<br>85<br>[261]   | unnilium<br>86<br>[262]    | unnilium<br>87<br>[266]   | unnilium<br>88<br>[269]  | unnilium<br>89<br>[264]  | unnilium<br>90<br>[269]  | unnilium<br>91<br>[268]  | unnilium<br>92<br>[271]  | unnilium<br>93<br>[276]  | unnilium<br>94<br>[275]  | unnilium<br>95<br>[279]  | unnilium<br>96<br>[274]  | unnilium<br>97<br>[278]  | unnilium<br>98<br>[273]  | unnilium<br>99<br>[277]  |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>83<br>[262]    | unnilium<br>84<br>[261]   | unnilium<br>85<br>[262]    | unnilium<br>86<br>[266]   | unnilium<br>87<br>[269]  | unnilium<br>88<br>[264]  | unnilium<br>89<br>[269]  | unnilium<br>90<br>[268]  | unnilium<br>91<br>[271]  | unnilium<br>92<br>[276]  | unnilium<br>93<br>[275]  | unnilium<br>94<br>[279]  | unnilium<br>95<br>[274]  | unnilium<br>96<br>[278]  | unnilium<br>97<br>[273]  | unnilium<br>98<br>[277]  |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>82<br>[262]    | unnilium<br>83<br>[261]   | unnilium<br>84<br>[262]    | unnilium<br>85<br>[266]   | unnilium<br>86<br>[269]  | unnilium<br>87<br>[264]  | unnilium<br>88<br>[269]  | unnilium<br>89<br>[268]  | unnilium<br>90<br>[271]  | unnilium<br>91<br>[276]  | unnilium<br>92<br>[275]  | unnilium<br>93<br>[279]  | unnilium<br>94<br>[274]  | unnilium<br>95<br>[278]  | unnilium<br>96<br>[273]  | unnilium<br>97<br>[277]  |
|  |   |   |   |   |   |   |   |    |    |    | unnilium<br>81<br>[262]    | unnilium<br>82<br>[261]   | unnilium<br>83<br>[262]    | unnilium<br>84<br>[266]   | unnilium<br>85<br>[269]  | unnilium<br>86<br>[264]  | unnilium<br>87<br>[269]  | unnilium<br>88<br>[268]  | unnilium<br>89<br>[271]  | unnilium<br>90<br>[276]  | unnilium<br>91<br>[275]  | unnilium<br>92<br>[279]  | unnilium<br>93<br>[274]  | unnilium<br>94<br>[278]  | unnilium<br>95           |                          |

# SOC Induced Mott Transition

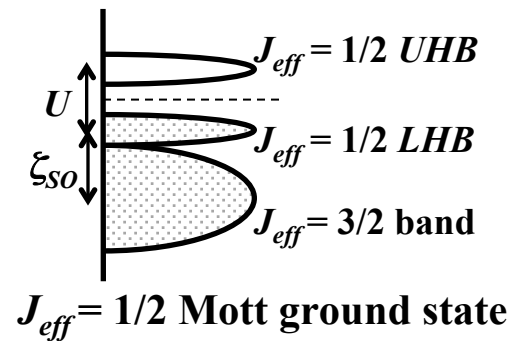
In cubic symmetry,



wide  $t_{2g}$ -band Metal



$J_{eff}$  band split due to SO



# $J_{eff}=1/2$ states

$t_{2g}$  maps onto  $p(l=1, s=1/2)$  manifold (TP equivalence)

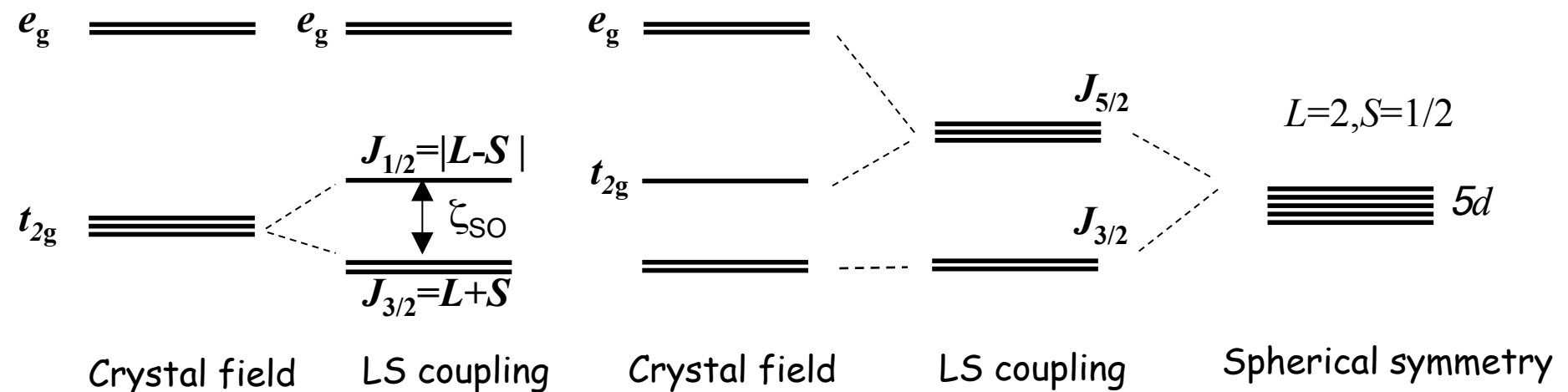
Taking only the  $t_{2g}$  subspace, angular momentum operator  $\mathbf{L}$  is given by

$$\begin{array}{c} xy \quad yz \quad zx \\ L_x = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad L_y = \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad L_z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix} \end{array}$$

which can be mapped onto  $\mathbf{L}=1$  manifold with

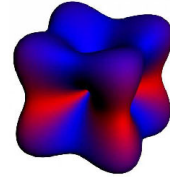
$$p_z \rightarrow xy, p_x \rightarrow yz, p_y \rightarrow zx$$

$$\mathbf{L}_{t_{2g}} \rightarrow -\mathbf{L}_p$$



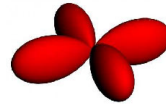
# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states

$J_{\text{eff}}=1/2$  states



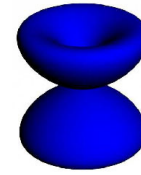
isospin up

=



spin up,  $l_z=0$

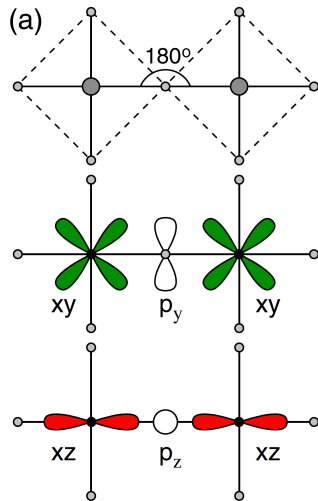
+



spin down,  $l_z=1$

$$|xy \uparrow\rangle + |yz \downarrow\rangle + i|zx \downarrow\rangle$$

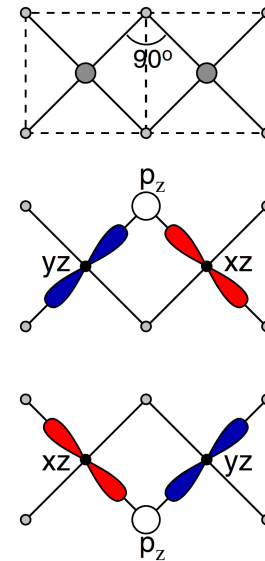
180° bond



Heisenberg

High-Tc superconductivity?

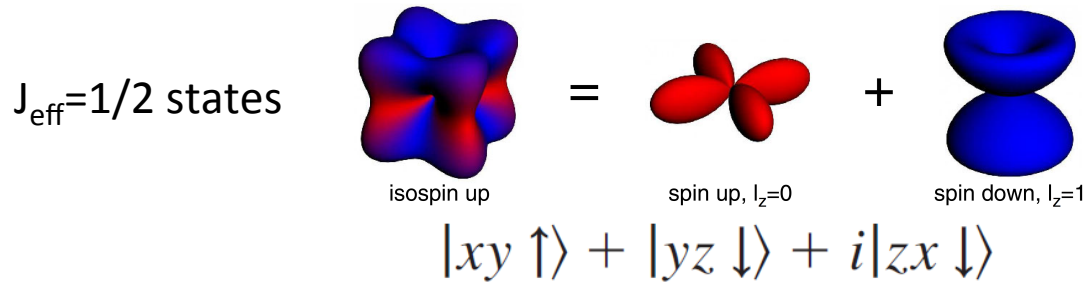
90° bond



complete suppression of Heisenberg

Kitaev spin liquid?

# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states



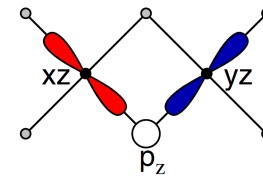
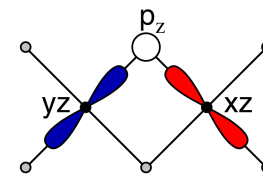
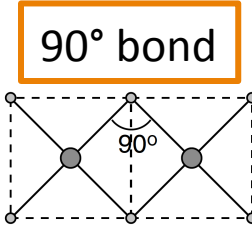
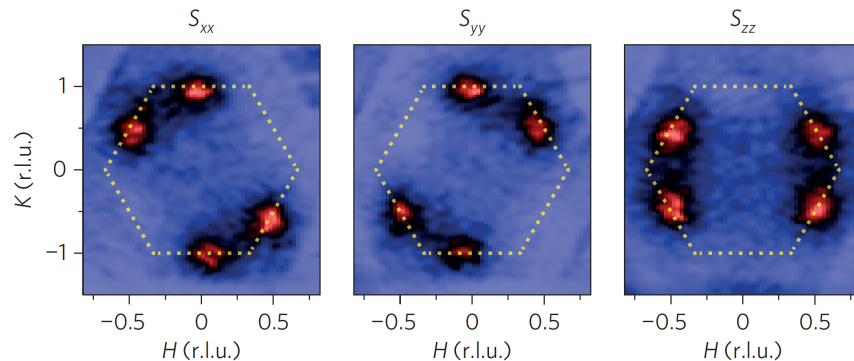
nature  
physics

LETTERS

PUBLISHED ONLINE: 11 MAY 2015 | DOI: 10.1038/NPHYS3322

## Direct evidence for dominant bond-directional interactions in a honeycomb lattice iridate $\text{Na}_2\text{IrO}_3$

Sae Hwan Chun<sup>1</sup>, Jong-Woo Kim<sup>2</sup>, Jungho Kim<sup>2</sup>, H. Zheng<sup>1</sup>, Constantinos C. Stoumpos<sup>1</sup>, C. D. Malliakas<sup>1</sup>, J. F. Mitchell<sup>1</sup>, Kavita Mehlawat<sup>3</sup>, Yogesh Singh<sup>3</sup>, Y. Choi<sup>2</sup>, T. Gog<sup>2</sup>, A. Al-Zein<sup>4</sup>, M. Moretti Sala<sup>4</sup>, M. Krisch<sup>4</sup>, J. Chaloupka<sup>5</sup>, G. Jackeli<sup>6,7</sup>, G. Khaliullin<sup>6</sup> and B. J. Kim<sup>6\*</sup>



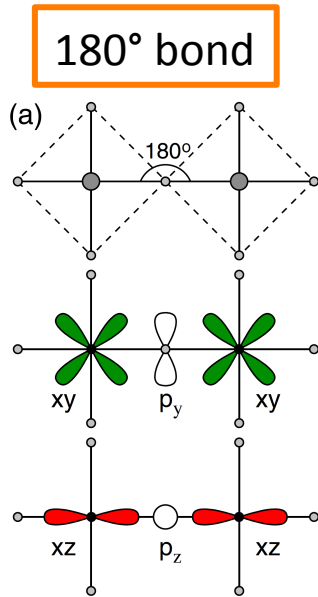
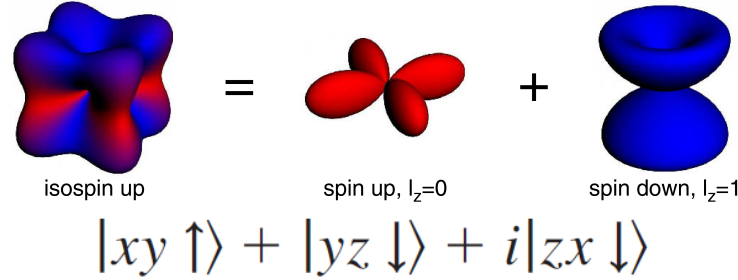
complete suppression of Heisenberg

Kitaev spin liquid?



# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states

$J_{\text{eff}}=1/2$  states



Heisenberg

High-Tc superconductivity?

## SUPERCONDUCTIVITY

# Fermi arcs in a doped pseudospin-1/2 Heisenberg antiferromagnet

Y. K. Kim,<sup>1</sup> O. Krupin,<sup>1</sup> J. D. Denlinger,<sup>1</sup> A. Bostwick,<sup>1</sup> E. Rotenberg,<sup>1</sup> Q. Zhao,<sup>2</sup> J. F. Mitchell,<sup>2</sup> J. W. Allen,<sup>3</sup> B. J. Kim<sup>2,3,4\*</sup>

[arXiv.org > cond-mat > arXiv:1506.06639](https://arxiv.org/cond-mat/1506.06639)

Condensed Matter > Strongly Correlated Electrons

## Observation of a $d$ -wave gap in electron-doped $\text{Sr}_2\text{IrO}_4$

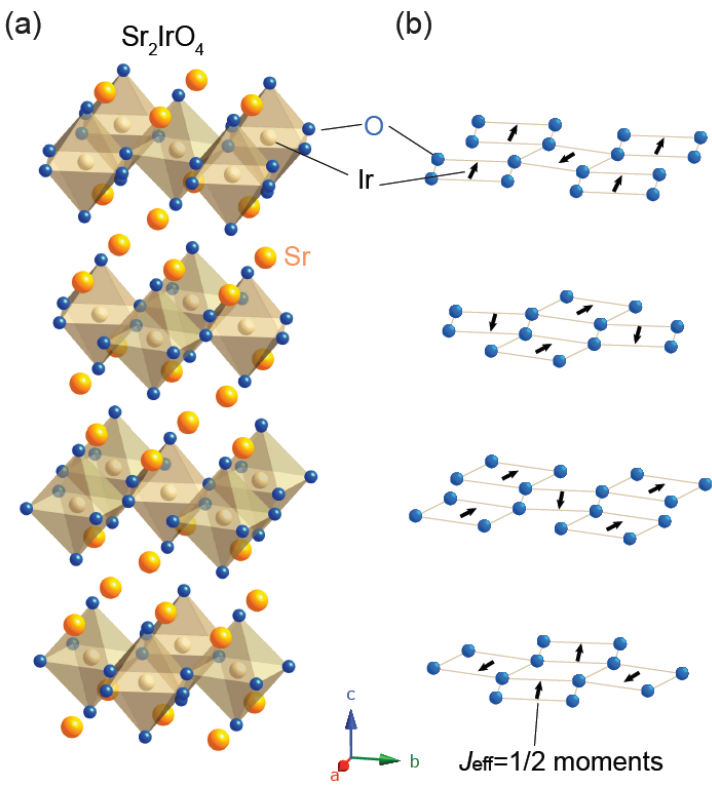
Y. K. Kim, N. H. Sung, J. D. Denlinger, B. J. Kim

(Submitted on 22 Jun 2015 (v1), last revised 25 Jun 2015 (this version, v2))

High temperature superconductivity in cuprates emerges out of a highly enigmatic 'pseudogap' metal phase. The mechanism of high temperature superconductivity is likely encrypted in the elusive relationship between the two phases, which spectroscopically is manifested as Fermi arcs---disconnected segments of zero-energy states---collapsing into  $d$ -wave point nodes upon entering the superconducting phase. Here, we reproduce this distinct cuprate phenomenology in the  $5d$  transition-metal oxide  $\text{Sr}_2\text{IrO}_4$ . Using angle-resolved photoemission, we show that clean, low-temperature phase of 6-8% electron-doped  $\text{Sr}_2\text{IrO}_4$  has gapless excitations only at four isolated points in the Brillouin zone with a predominant  $d$ -wave symmetry of the gap. Our work thus establishes a connection between the low-temperature  $d$ -wave instability and the previously reported high-temperature Fermi arcs in electron-doped  $\text{Sr}_2\text{IrO}_4$ . Although the physical origin of the  $d$ -wave gap remains to be understood,  $\text{Sr}_2\text{IrO}_4$  is a first non-cuprate material to spectroscopically reproduce the complete phenomenology of the cuprates, thus offering a new material platform to investigate the relationship between the pseudogap and the  $d$ -wave gap.

# Ruddelsden-Popper Series Iridates

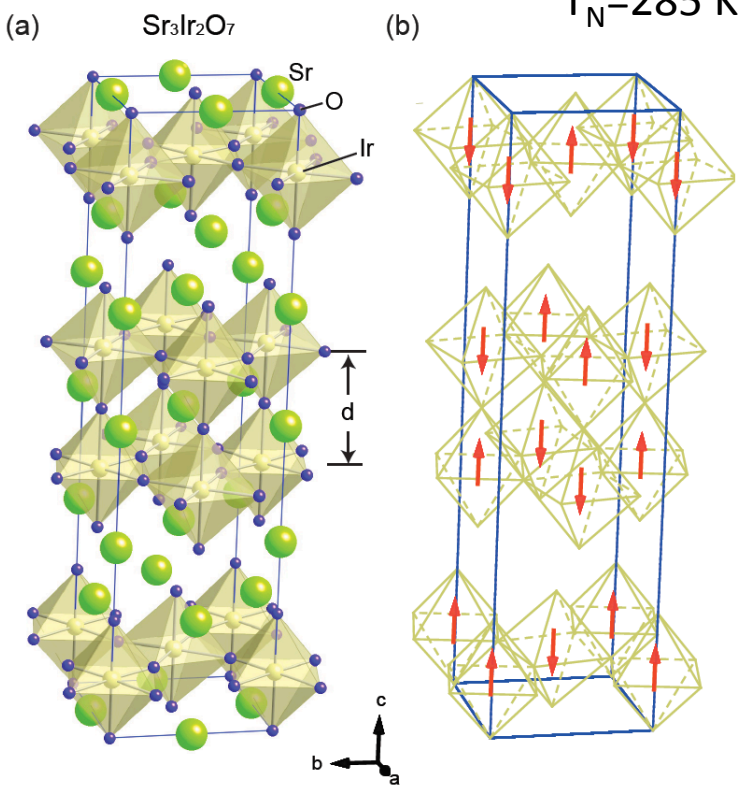
$\text{Sr}_2\text{IrO}_4$   $T_N=240$  K



canted AF with  
in-plane moments

B. J. Kim et al. Science (2009)

$\text{Sr}_3\text{Ir}_2\text{O}_7$   $T_N=285$  K



G-type AF  
c-axis collinear

J. -W. Kim, BJK et al. PRL (2012),  
S. Boseggia et al, J. Phys. Condens. Matter (2015)  
J. P. Clancy et al., arxiv (2012)  
S. Fujiyama et al. PRB (2012)

# Resonant x-ray scattering

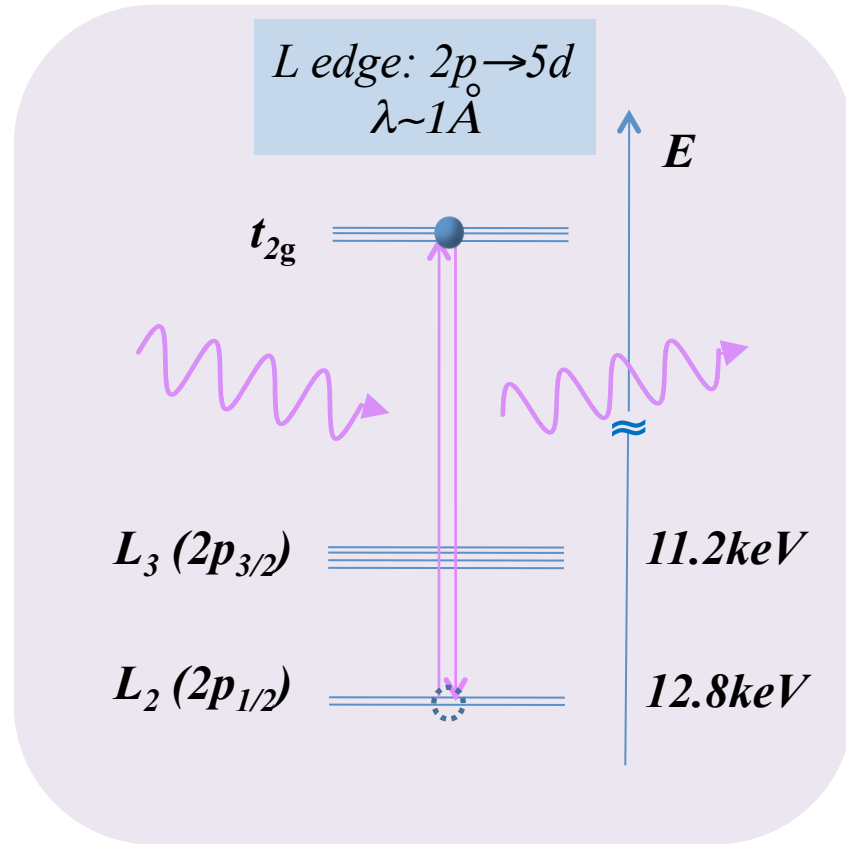
Direct probe for the 5d state responsible for magnetism

$$H' = \frac{e^2}{2m_e c^2} \sum_i A(\mathbf{r}_i)^2 - \frac{e^2 \hbar}{2m_e^2 c^4} \sum_i \mathbf{s}_i \cdot \left( \frac{\partial \mathbf{A}}{\partial t} \times \mathbf{A} \right) - \frac{e}{m_e c} \sum_i \mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p} - \frac{e^2 \hbar}{2m_e^2 c^4} \sum_i \mathbf{s}_i \cdot (\nabla \times \mathbf{A}(\mathbf{r}_i))$$

$$F_{E1}^{(reso)} = \frac{e^2}{m_e c^2} \sum_{n,m} e^{i\mathbf{K} \cdot (\mathbf{n} + d_m)} \sum_{\alpha\beta} \varepsilon'_\alpha \varepsilon_\beta f_m^{\alpha\beta}$$

$$f_m^{\alpha\beta} = \sum_c \frac{m_e \omega_{ca}^3}{\omega} \frac{\langle a | R_m^\alpha | c \rangle \langle c | R_m^\beta | a \rangle}{\hbar\omega - \hbar\omega_{ac} + i\Gamma/2}$$

Cartesian tensor of rank 2



# Resonant x-ray scattering and x-ray absorption

-Related through the optical theorem

$$\begin{aligned} F_{\boldsymbol{\epsilon}_{in}\boldsymbol{\epsilon}_{out}} &= F^{(0)}(\boldsymbol{\epsilon}_{in} \cdot \boldsymbol{\epsilon}_{out}^*) && \text{charge} \\ &+ F^{(1)}(\boldsymbol{\epsilon}_{in} \times \boldsymbol{\epsilon}_{out}^* \cdot \hat{\mathbf{m}}) && \text{magnetic dipole} \\ &+ F^{(2)}((\boldsymbol{\epsilon}_{out}^* \cdot \hat{\mathbf{m}})(\boldsymbol{\epsilon}_{in} \cdot \hat{\mathbf{m}}) - \frac{1}{3}(\boldsymbol{\epsilon}_{in} \cdot \boldsymbol{\epsilon}_{out}^*)) && \text{electric quadrupole} \end{aligned}$$

$F0$ , describes the isotropic absorption

$F1$ , describes the XMCD spectra

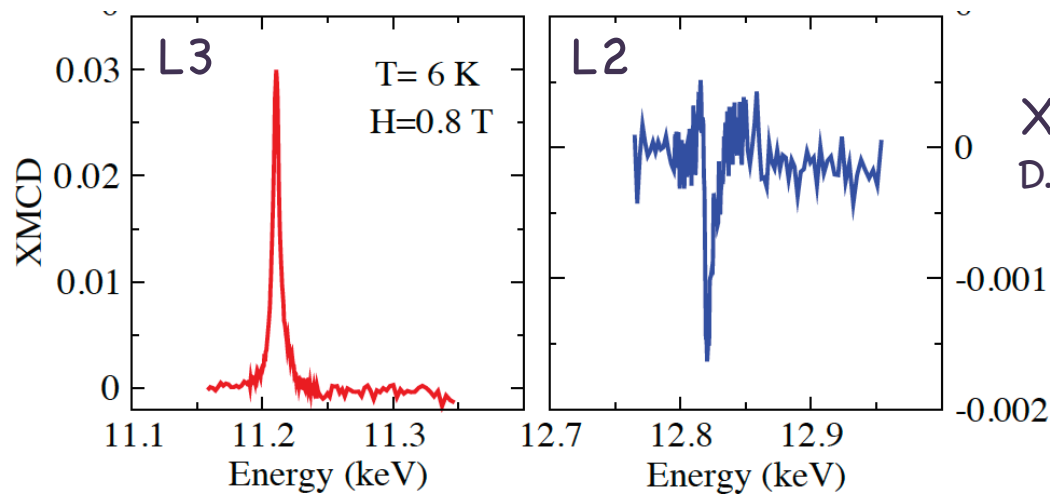
$F2$ , describes the XMLD spectra

G. van der Laan, J. Phys. Soc. Jpn. 63, 2393 (1994)

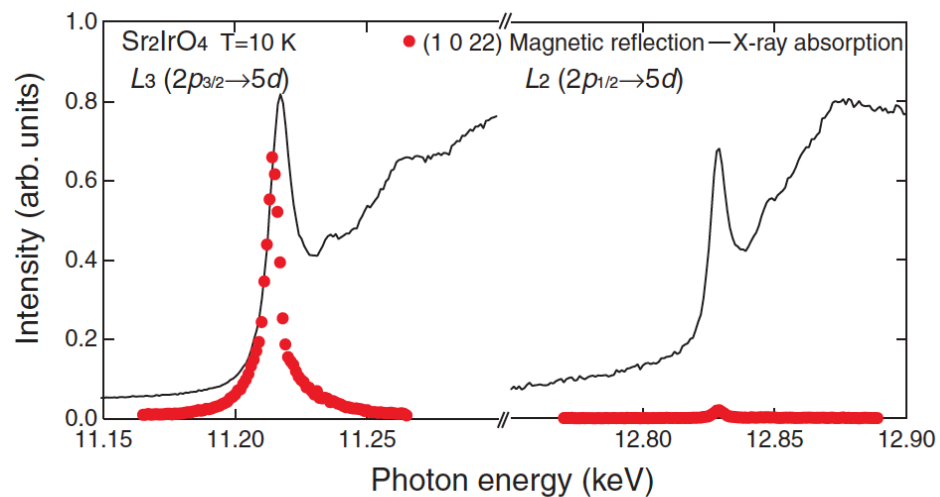
M. Haverkort, PRL 105, 167404 (2010)

Resonant x-ray scattering contains information about spin and orbital structure of scattering ion

# XMCD and RXD on $\text{Sr}_2\text{IrO}_4$

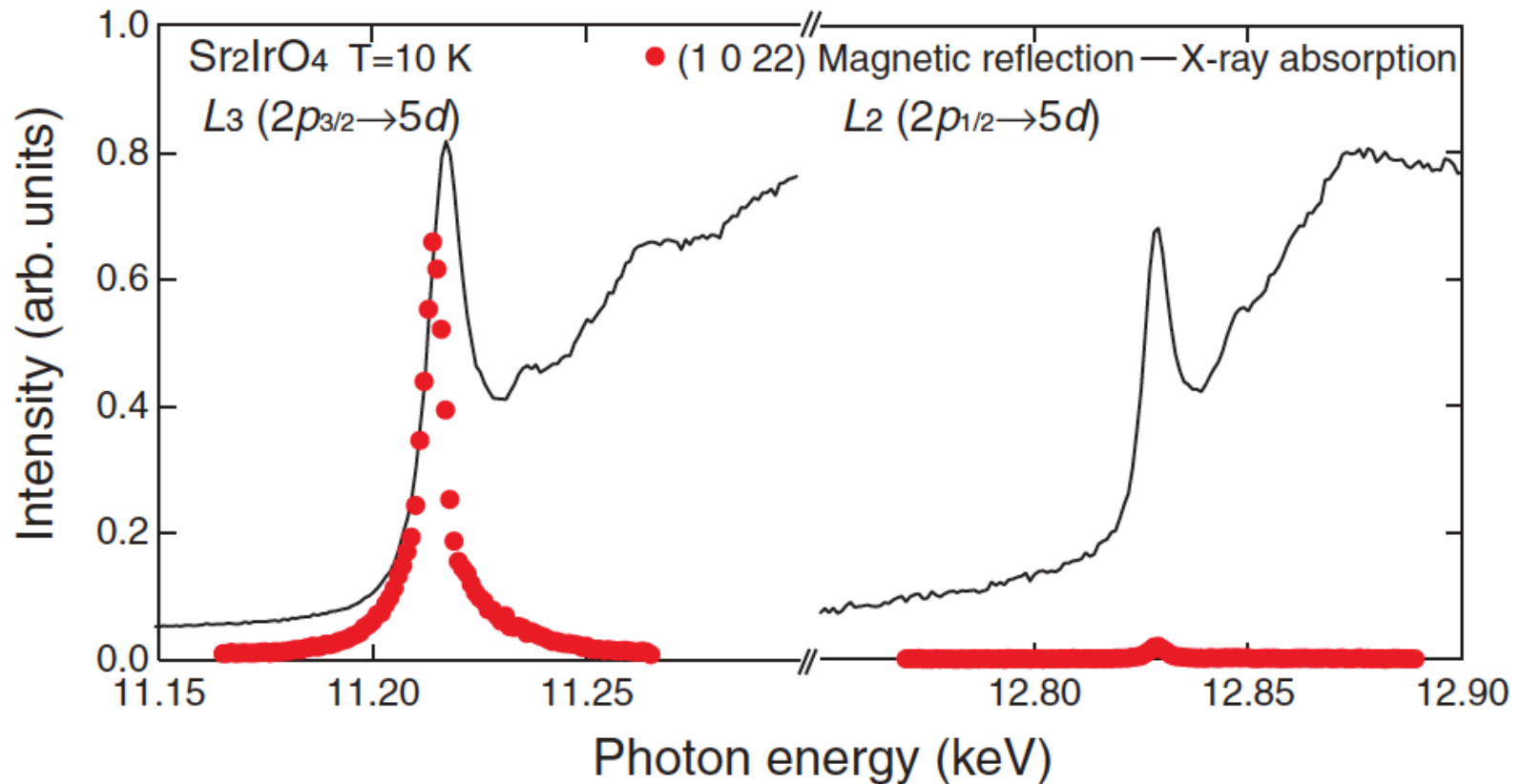


XMCD  
D. Haskel et al. PRL (2012)



RXD  
B. J. Kim et al. Science (2009)

# Evidence for $J_{\text{eff}}=1/2$ states



Almost no resonance at  $L_2$ :

$L_2$  scattering intensity is only about 1% of that of the  $L_3$ .

# RIXS cross section

To calculate  $O_{l_z, l_z'}^{\alpha\beta} = \sum_{j_z} \langle l, l_z | R^\alpha | j, j_z \rangle \langle j, j_z | R^\beta | l, l_z' \rangle$

we need  $\langle l, l_z | T_q^k | j, j_z' \rangle$

→ Spherical tensor of rank 1

$$z = T_0^1$$

$$x = -\frac{1}{\sqrt{2}}(T_1^1 - T_{-1}^1)$$

$$y = \frac{1}{\sqrt{2}i}(T_1^1 + T_{-1}^1)$$

$$\langle l = 2, s = 1/2; l_z, s_z | T_q^k | l' = 1, s' = 1/2; j, j_z' \rangle$$

$$= \sum_{l_z', s_z'} \langle l = 2, s = 1/2; l_z, s_z | T_q^k | l' = 1, s' = 1/2; l_z', s_z' \rangle \langle l' = 1, s' = 1/2; l_z', s_z' | j, j_z' \rangle$$

$$= \sum_{l_z', s_z'} \langle l, s; l_z, s_z | T_q^k | l', s'; l_z', s_z' \rangle \delta_{s_z s_z'} \langle l', s'; l_z', s_z' | j, j_z' \rangle$$

Clebsch-Gordan Coefficient

Wigner-Eckart theorem

$$\propto \sum_{l_z'} \langle l, k; l_z', q | j, j_z \rangle \langle l', s'; l_z', s_z | j, j_z \rangle$$

$$\langle l, l_z | T_q^k | l', l_z' \rangle = \langle l, k; l_z', q | l, k; l, l_z \rangle \frac{\langle l' || T^k || l \rangle}{\sqrt{2l+1}}$$

$J_{\text{eff}}=1/2 \rightarrow$  Experiment  
Yes!

Experiment  $\overset{?}{\rightarrow} J_{\text{eff}}=1/2$



## FAST TRACK COMMUNICATION

# The magnetic motif and the wavefunction of Kramers ions in strontium iridate ( $\text{Sr}_2\text{IrO}_4$ )

L C Chapon<sup>1</sup> and S W Lovesey<sup>1,2</sup>PRL **112**, 026403 (2014)

PHYSICAL REVIEW LETTERS

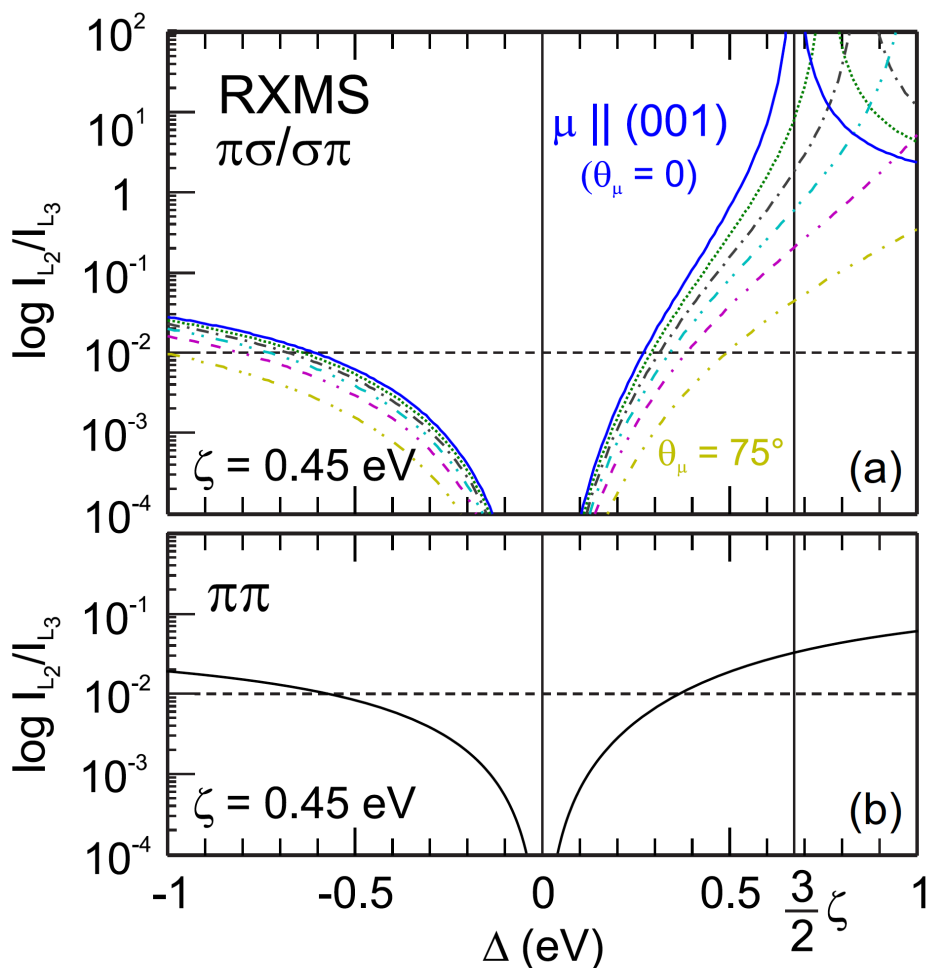
week ending  
17 JANUARY 2014

## Resonant X-Ray Scattering and the $j_{\text{eff}} = 1/2$ Electronic Ground State in Iridate Perovskites

M. Moretti Sala,<sup>1,\*</sup> S. Boseggia,<sup>2,3</sup> D. F. McMorrow,<sup>2,4</sup> and G. Monaco<sup>1</sup>

## Resonant X-Ray Scattering and the $j_{\text{eff}} = 1/2$ Electronic Ground State in Iridate Perovskites

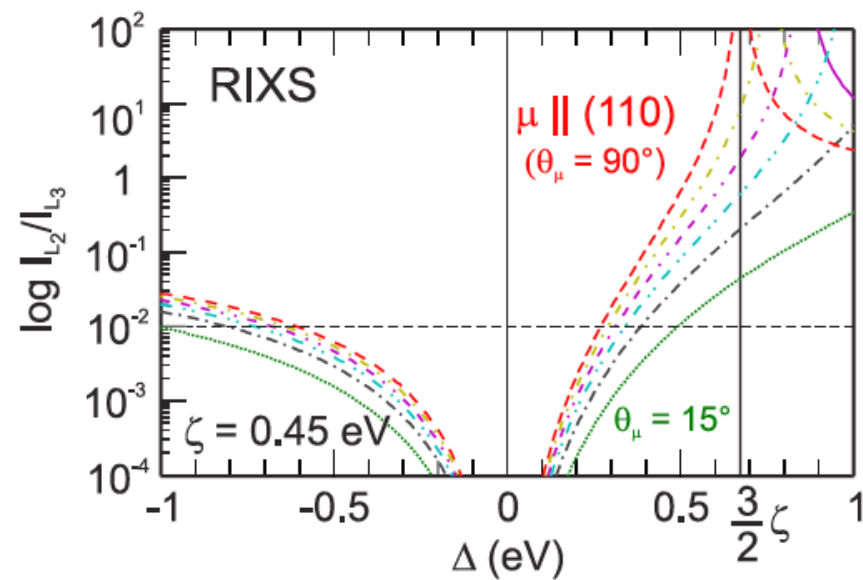
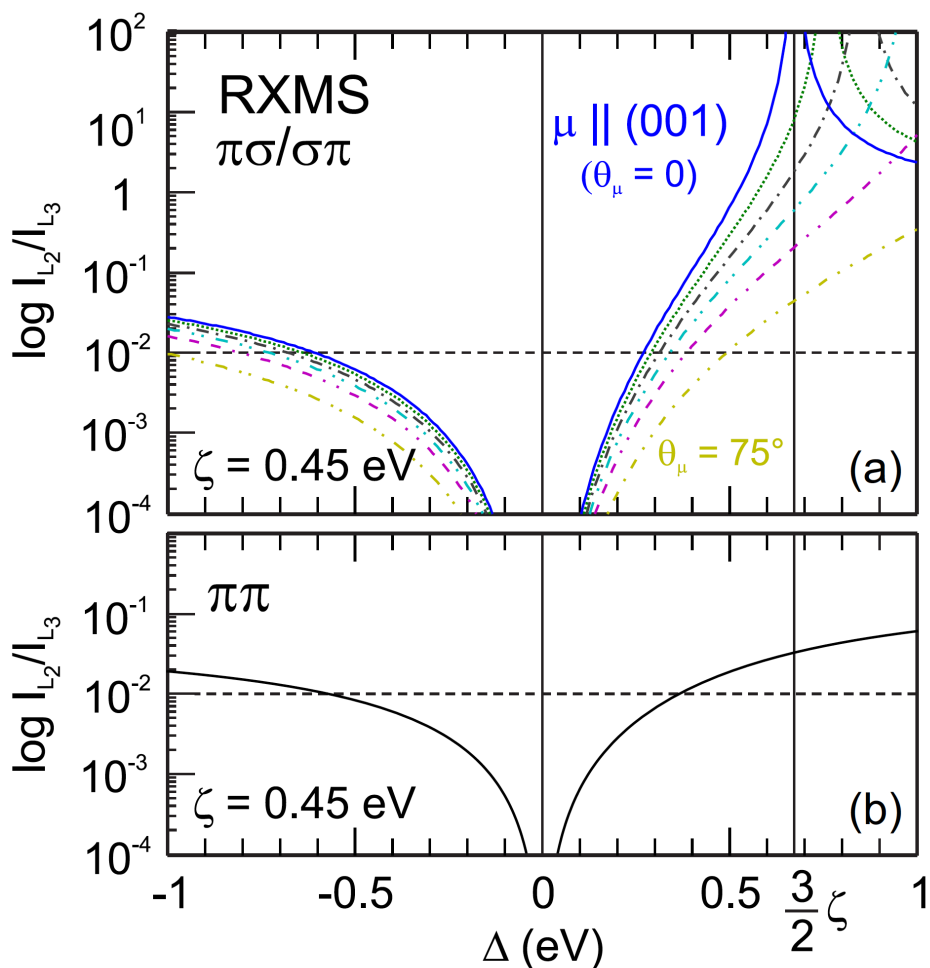
M. Moretti Sala,<sup>1,\*</sup> S. Boseggia,<sup>2,3</sup> D. F. McMorrow,<sup>2,4</sup> and G. Monaco<sup>1</sup>



- valid only if  $M$  is along the axis of distortion (c-axis)
- $L_2$  intensity vanishes for any  $\Delta$  if  $M$  is in the ab-plane

# Resonant X-Ray Scattering and the $j_{\text{eff}} = 1/2$ Electronic Ground State in Iridate Perovskites

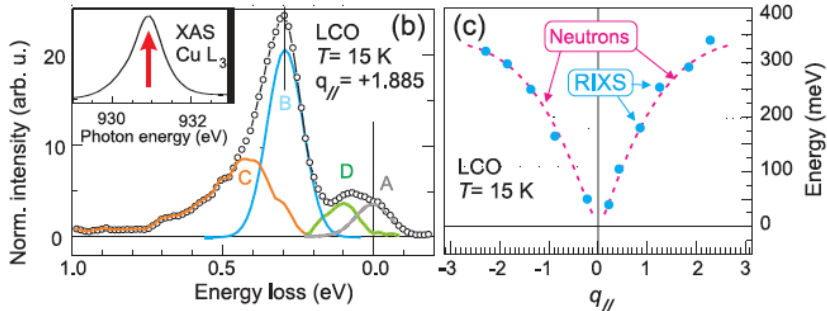
M. Moretti Sala,<sup>1,\*</sup> S. Boseggia,<sup>2,3</sup> D. F. McMorrow,<sup>2,4</sup> and G. Monaco<sup>1</sup>



# RIXS: New Tool to study Magnetic Excitations

soft x-ray (<1 keV)

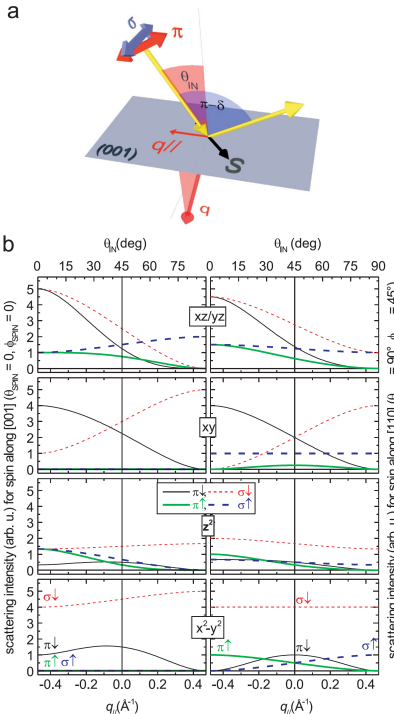
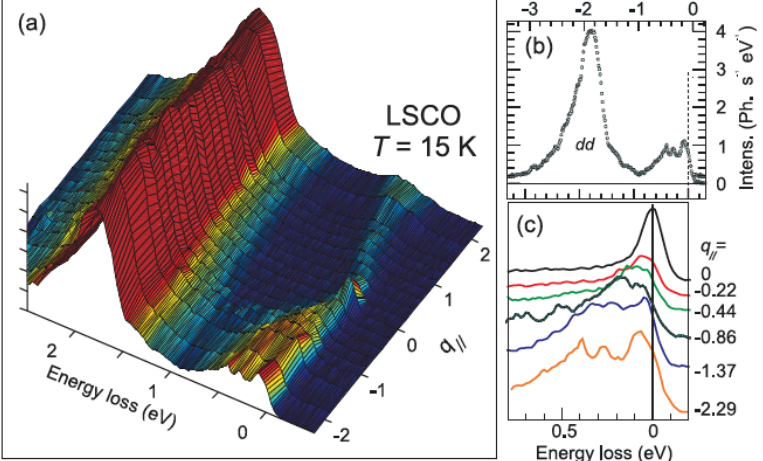
RIXS experiment on thin film of  $\text{La}_2\text{CuO}_4$



## Theoretical Demonstration of How the Dispersion of Magnetic Excitations in Cuprate Compounds can be Determined Using Resonant Inelastic X-Ray Scattering

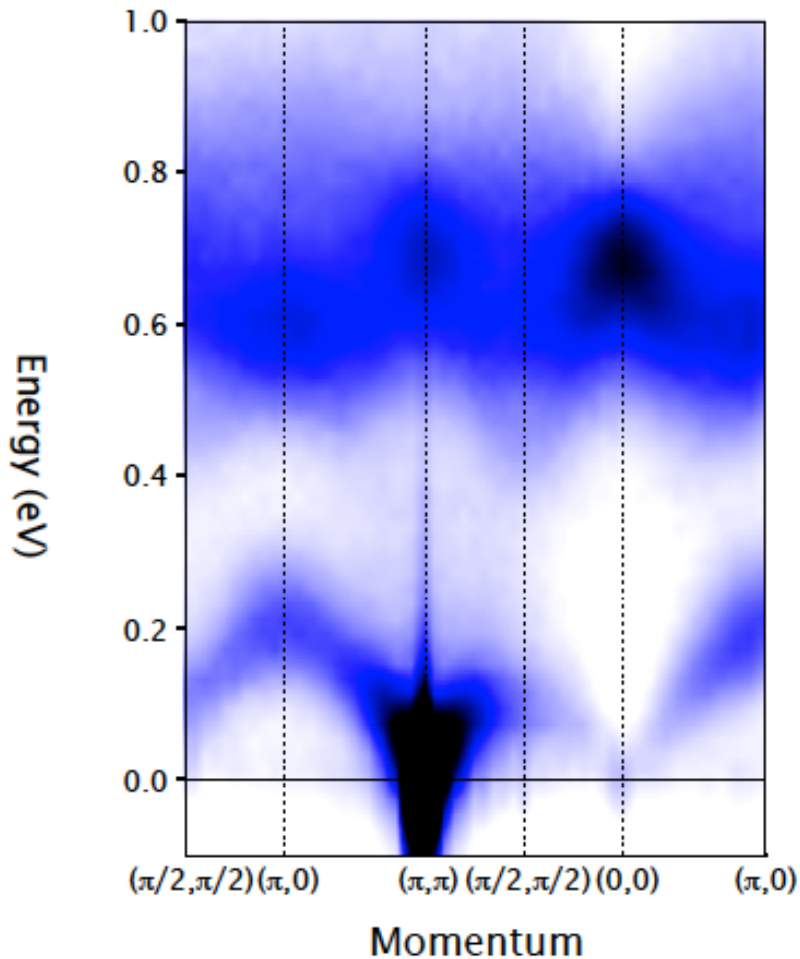
Luuk J. P. Ament,<sup>1,4</sup> Giacomo Ghiringhelli,<sup>2</sup> Marco Moretti Sala,<sup>2</sup> Lucio Braicovich,<sup>2</sup> and Jeroen van den Brink<sup>1,3,4</sup>  
<sup>1</sup>Institute-Lorentz for Theoretical Physics, Universiteit Leiden, 2300 RA Leiden, The Netherlands  
<sup>2</sup>INFM/CNR Coherentia and Soft-Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy  
<sup>3</sup>Institute for Molecules and Materials, Radboud Universiteit, 6500 GL Nijmegen, The Netherlands  
<sup>4</sup>Stanford Institute for Materials and Energy Sciences, Stanford University and SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA  
 (Received 13 March 2009; published 11 September 2009)

We show that in resonant inelastic x-ray scattering (RIXS) at the copper  $L$  and  $M$  edge direct spin-flip scattering is in principle allowed. We demonstrate how this possibility can be exploited to probe the dispersion of magnetic excitations, for instance magnons, of cuprates such as the high  $T_c$  superconductors. We compute the relevant local and momentum dependent magnetic scattering amplitudes, which we compare to the elastic and  $dd$ -excitation scattering intensities. For cuprates these theoretical results put RIXS as a technique on the same footing as neutron scattering.



L. Braicovich et al., PRL (2010)

# RIXS: New Tool to study Magnetic Excitations



5d TMO hard x-ray ( $\sim 11$  keV)

2010

our first experiment on iridate  
using Si (844) analyzer @ APS  
130 meV, 3000 cps

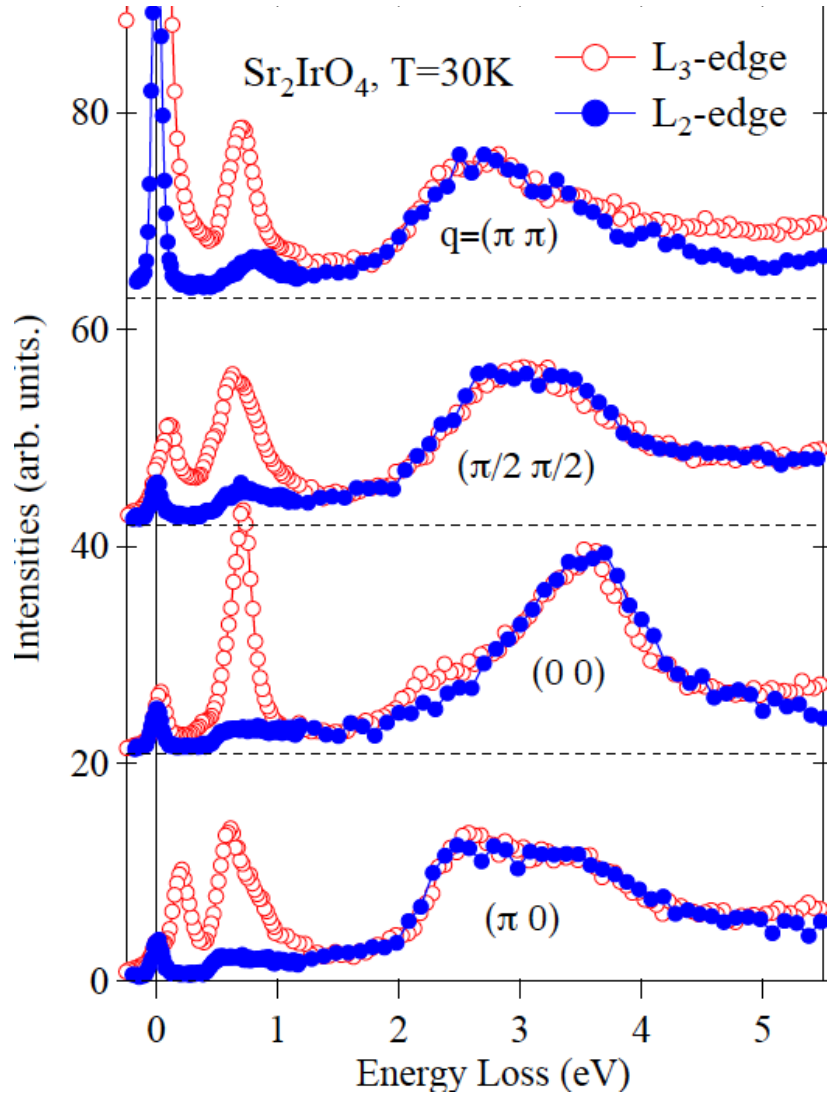
now

25 meV resolution routinely  
available at APS and ESRF

2016

sub 10-meV targeted in  
coming years

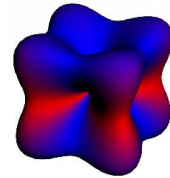
# L2/L3 intensity ratio in RIXS



magnon at L2 edge suppressed below detection level!

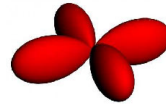
# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states

$J_{\text{eff}}=1/2$  states



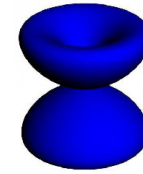
isospin up

=



spin up,  $l_z=0$

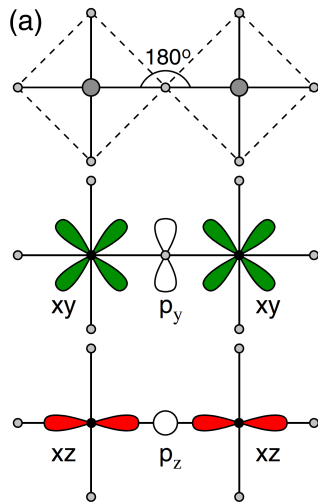
+



spin down,  $l_z=1$

$$|xy \uparrow\rangle + |yz \downarrow\rangle + i|zx \downarrow\rangle$$

180° bond

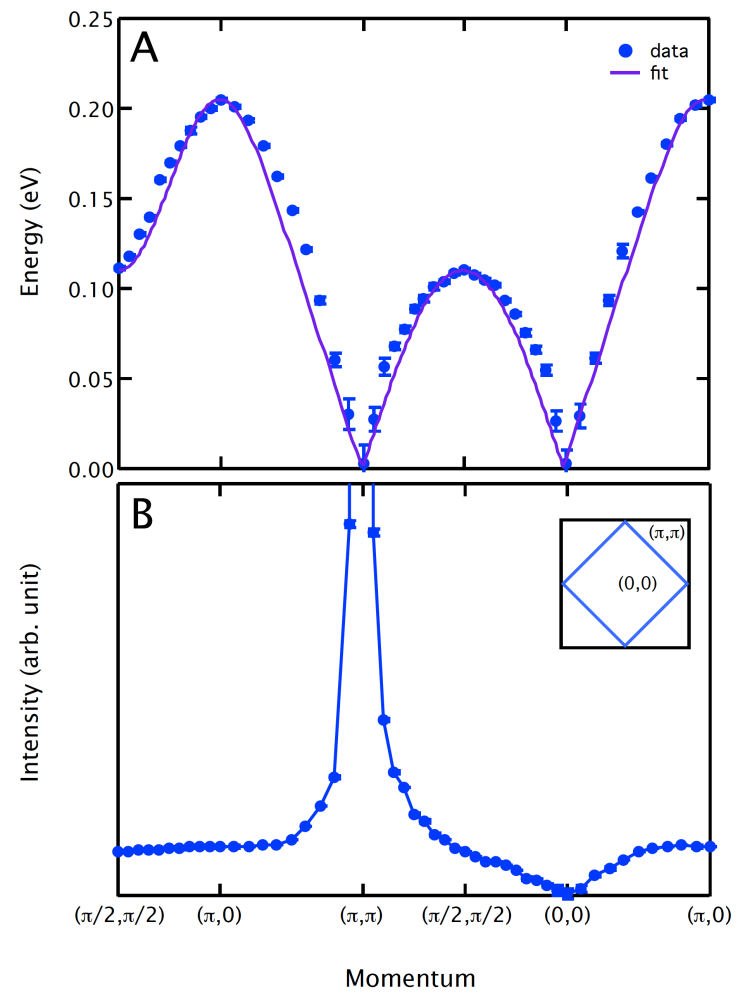
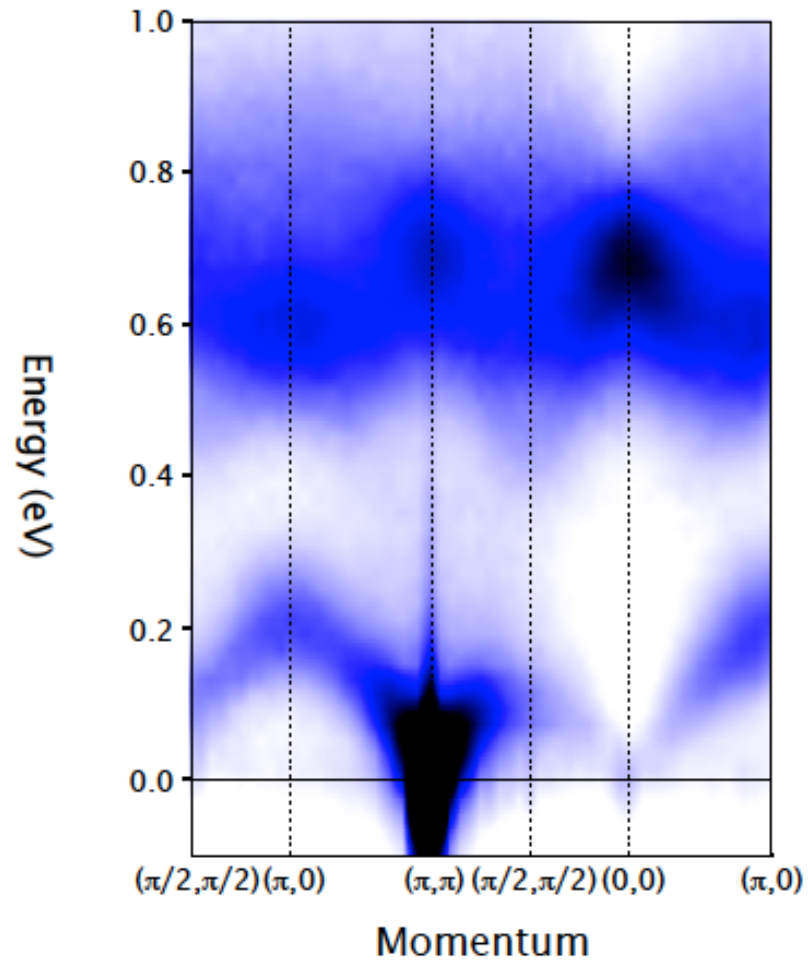


$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j),$$

Predominantly  
Heisenberg-like  
 $J_1 \gg J_2$

# Spin wave- fitting to Heisenberg model

2010

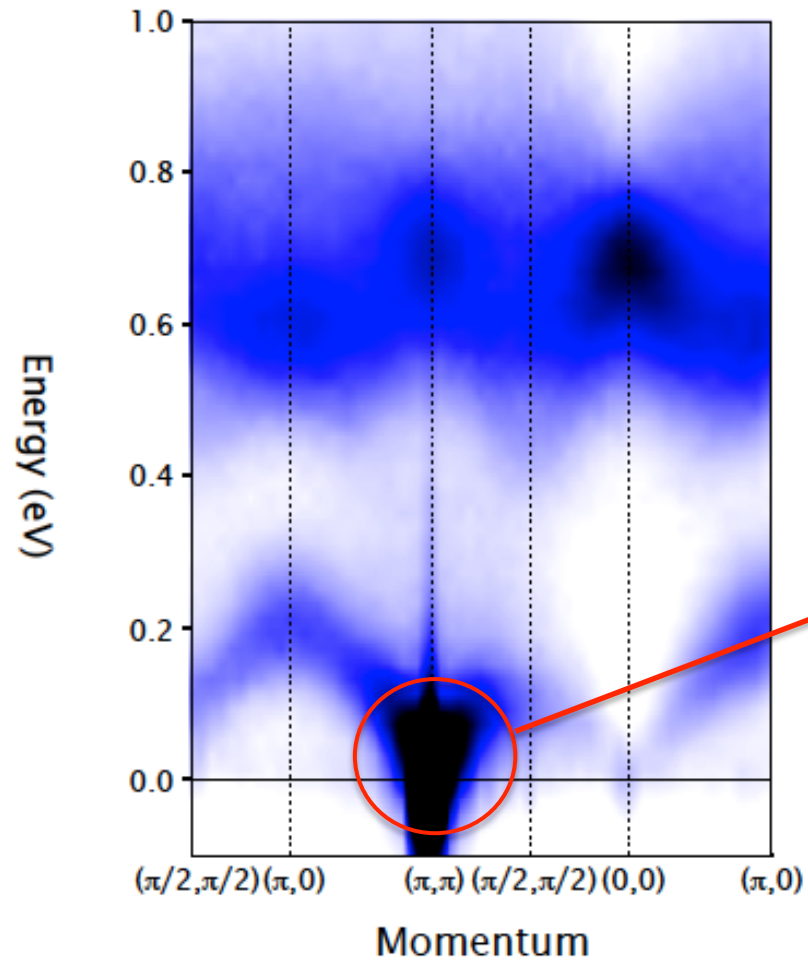


$J=60$   
 $J'=-20$   
 $J''=15$

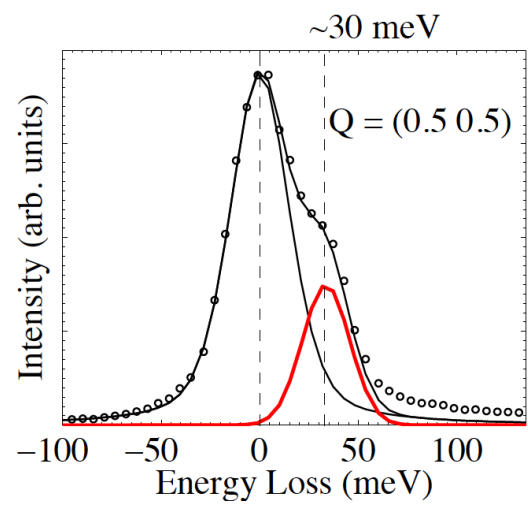


# Spin wave gap

2010



2015

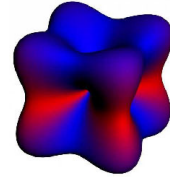


Sizable XY anisotropy!

see also J. Vale et al. PRB (2015)

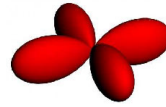
# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states

$J_{\text{eff}}=1/2$  states



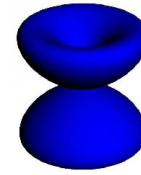
isospin up

=



spin up,  $l_z=0$

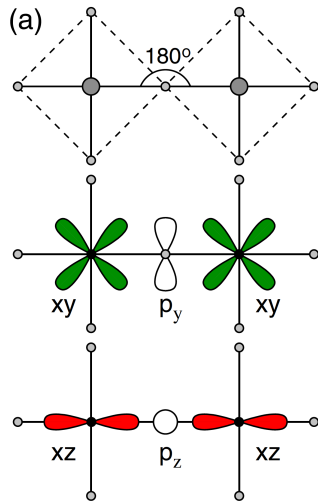
+



spin down,  $l_z=1$

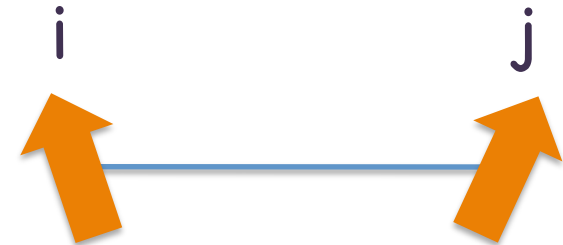
$$|xy \uparrow\rangle + |yz \downarrow\rangle + i|zx \downarrow\rangle$$

180° bond



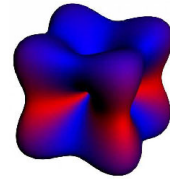
$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j),$$

- Compass
- bond-directional
- Pseudodipolar



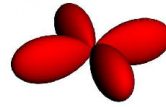
# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states

$J_{\text{eff}}=1/2$  states



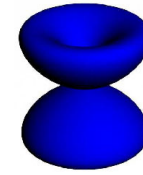
isospin up

=



spin up,  $l_z=0$

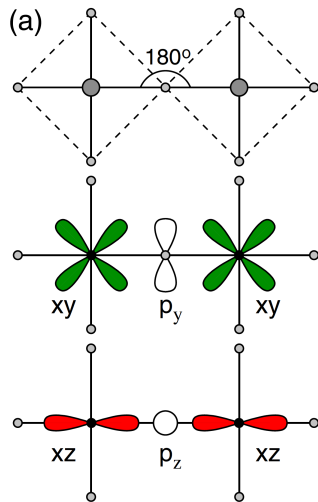
+



spin down,  $l_z=1$

$$|xy \uparrow\rangle + |yz \downarrow\rangle + i|zx \downarrow\rangle$$

180° bond



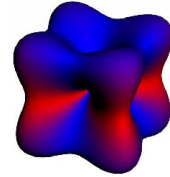
$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j),$$

- Compass
- bond-directional
- Pseudodipolar



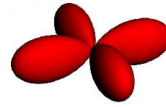
# Goodenough-Kanamori theory on $J_{\text{eff}}=1/2$ states

$J_{\text{eff}}=1/2$  states



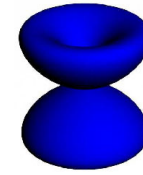
isospin up

=



spin up,  $l_z=0$

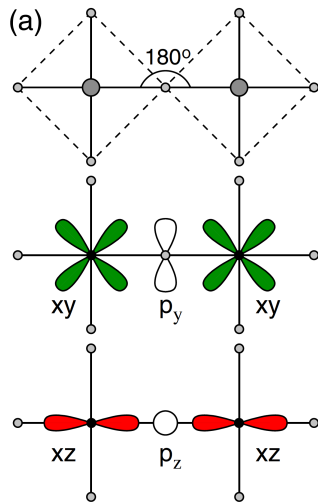
+



spin down,  $l_z=1$

$$|xy \uparrow\rangle + |yz \downarrow\rangle + i|zx \downarrow\rangle$$

180° bond



$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j),$$

- Compass
- bond-directional
- Pseudodipolar

responsible for  
magnetic anisotropy  
and magnon gap

weak SOC limit: scales with  $\lambda$   
strong SOC limit: scales with  $J_H/U$

# Pseudodipolar term in a square lattice

$x$



$$\mathcal{H}_{ij} = J_{ij} \vec{S}_i \cdot \vec{S}_j + \Gamma S_i^x S_j^x$$

$$\frac{\Gamma}{2} (S_i^x S_j^x + S_i^y S_j^y) + \frac{\Gamma}{2} (S_i^x S_j^x - S_i^y S_j^y)$$

$A_{1g}$

$B_{1g}$

$y$

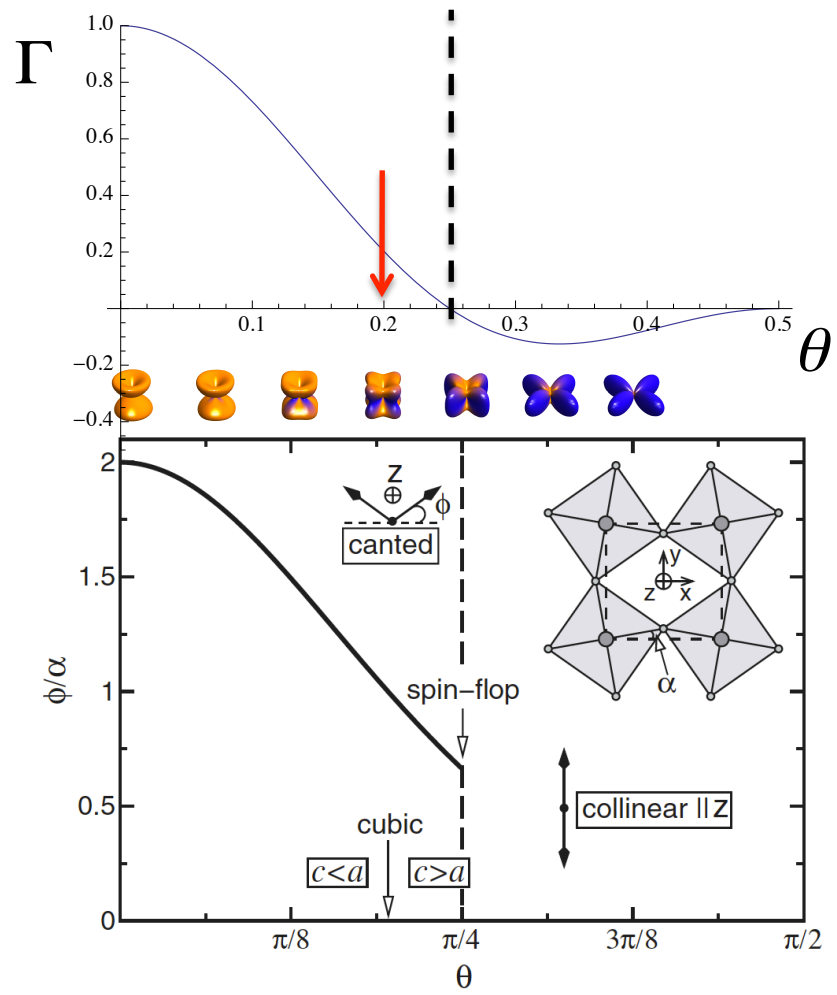


$$\mathcal{H}_{ij} = J_{ij} \vec{S}_i \cdot \vec{S}_j + \Gamma S_i^y S_j^y$$

$$\frac{\Gamma}{2} (S_i^x S_j^x + S_i^y S_j^y) - \frac{\Gamma}{2} (S_i^x S_j^x - S_i^y S_j^y)$$

$$\mathcal{H}_{ij} = (J_{ij} + \Gamma/2) \vec{S}_i \cdot \vec{S}_j - \frac{\Gamma}{2} S_i^z S_j^z$$

# Pseudodipolar term in a square lattice

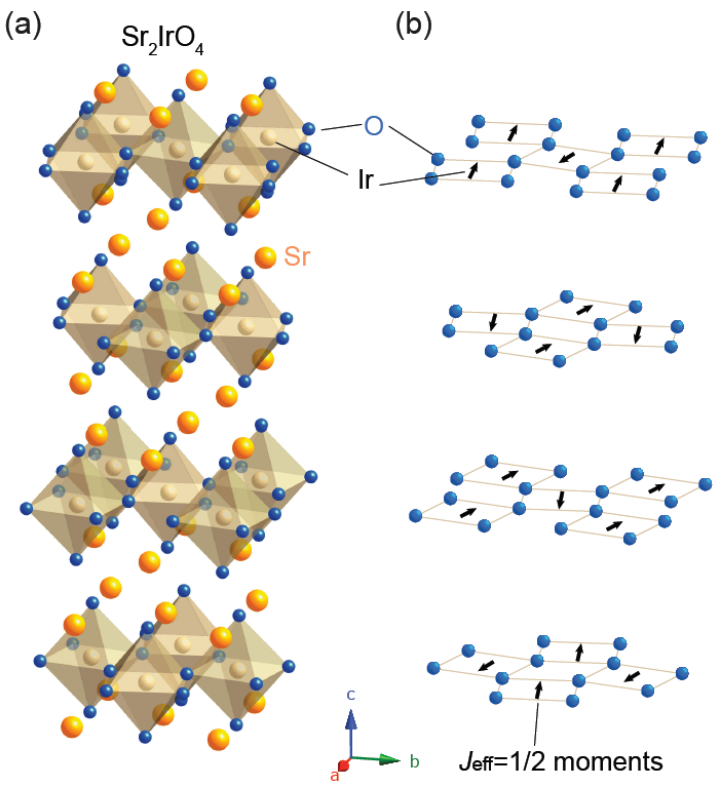


$$\mathcal{H}_{ij} = (J_{ij} + \Gamma/2)\vec{S}_i \cdot \vec{S}_j - \frac{\Gamma}{2}S_i^z S_j^z$$

# Ruddelsden-Popper Series Iridates



$T_N=240$  K

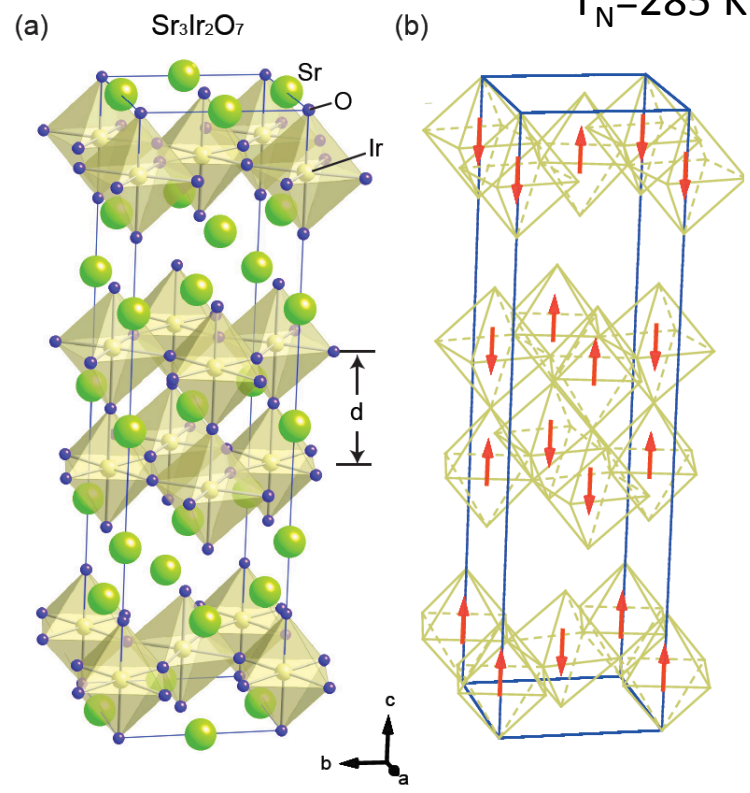


canted AF with  
in-plane moments

B. J. Kim et al. Science (2009)



$T_N=285$  K



G-type AF  
c-axis collinear

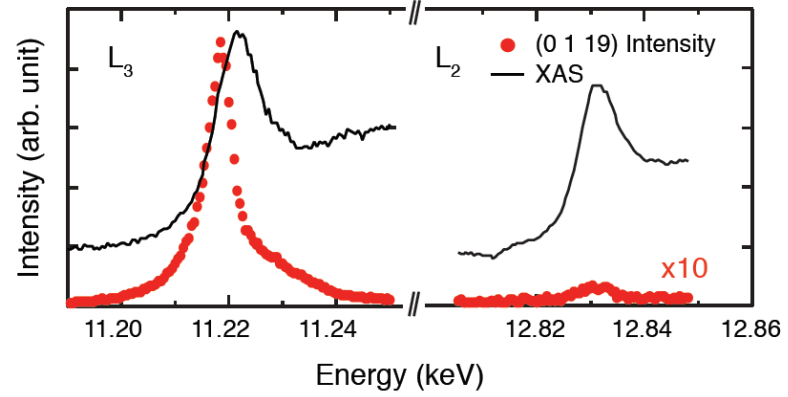
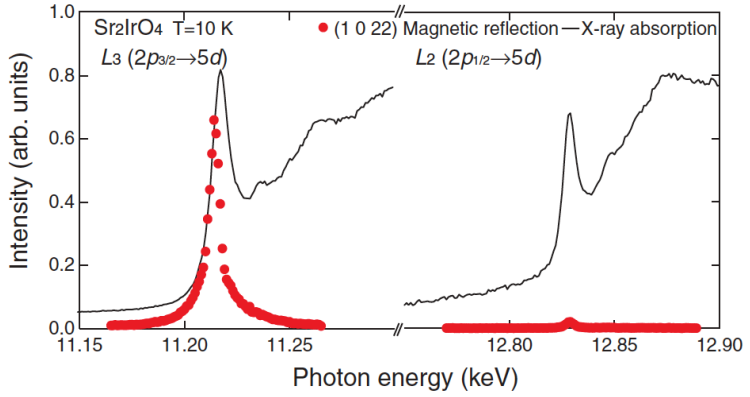
J. -W. Kim, BJK et al. PRL (2012),  
S. Boseggia et al, J. Phys. Condens. Matter (2015)  
J. P. Clancy et al., arxiv (2012)  
S. Fujiyama et al. PRB (2012)

# L2/L3 RXD Intensity

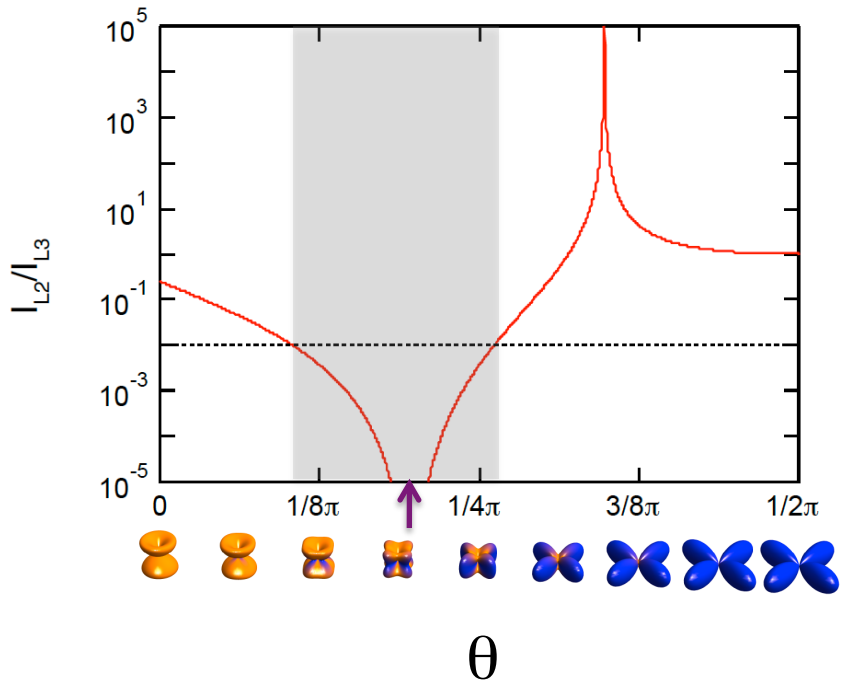


L3

L2



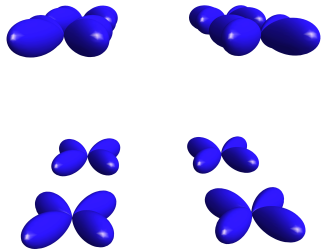
$I_{L2}/I_{L3} < 1\%$





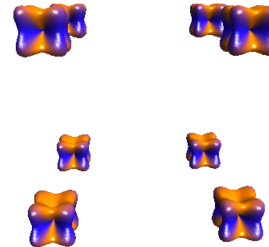
$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j),$$

Orbitals polarized,  
anisotropy in superexchange  
interactions



$$J_{ab} \gg J_c,$$

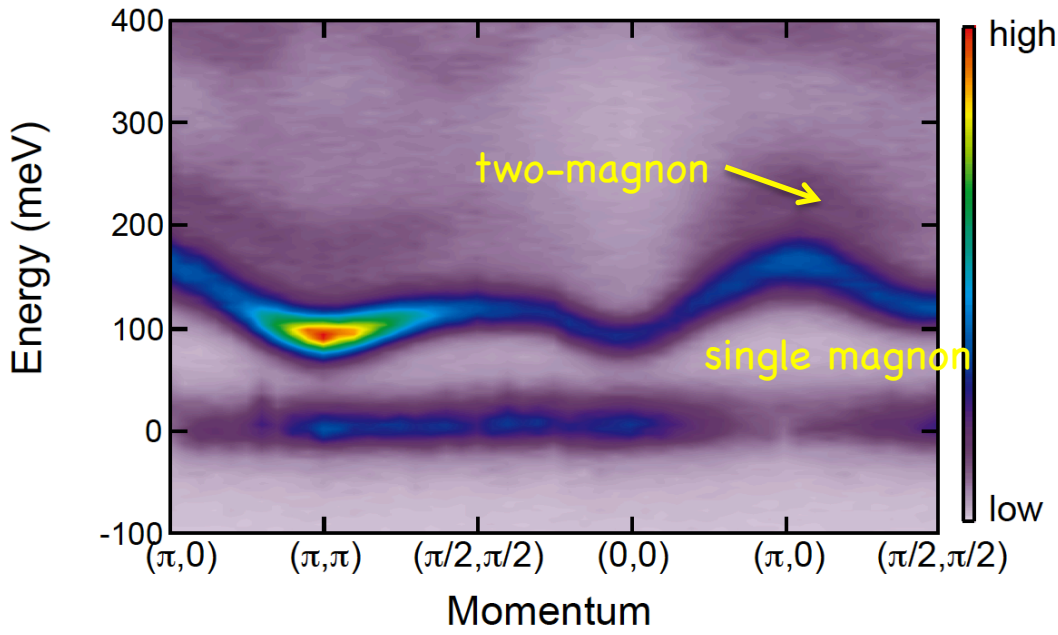
Superexchange interactions  
multidirectional



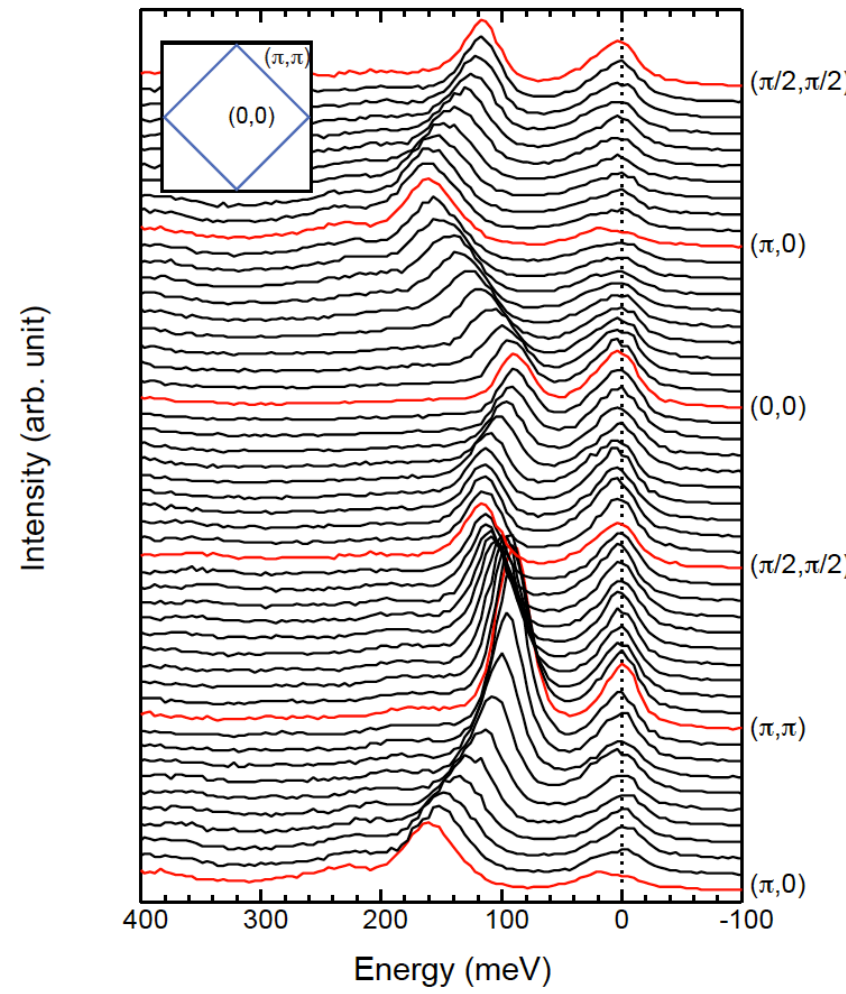
$$J_{ab} \approx J_c$$

# Giant Magnon Gap in $\text{Sr}_3\text{Ir}_2\text{O}_7$

$q_c = \pi/3$



- Large magnon gap  $\Delta_m \approx 90$  meV
- Total magnon bandwidth  $\approx 70$  meV

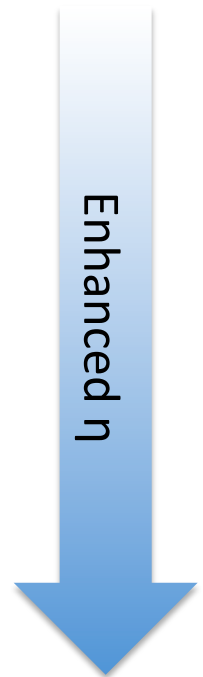
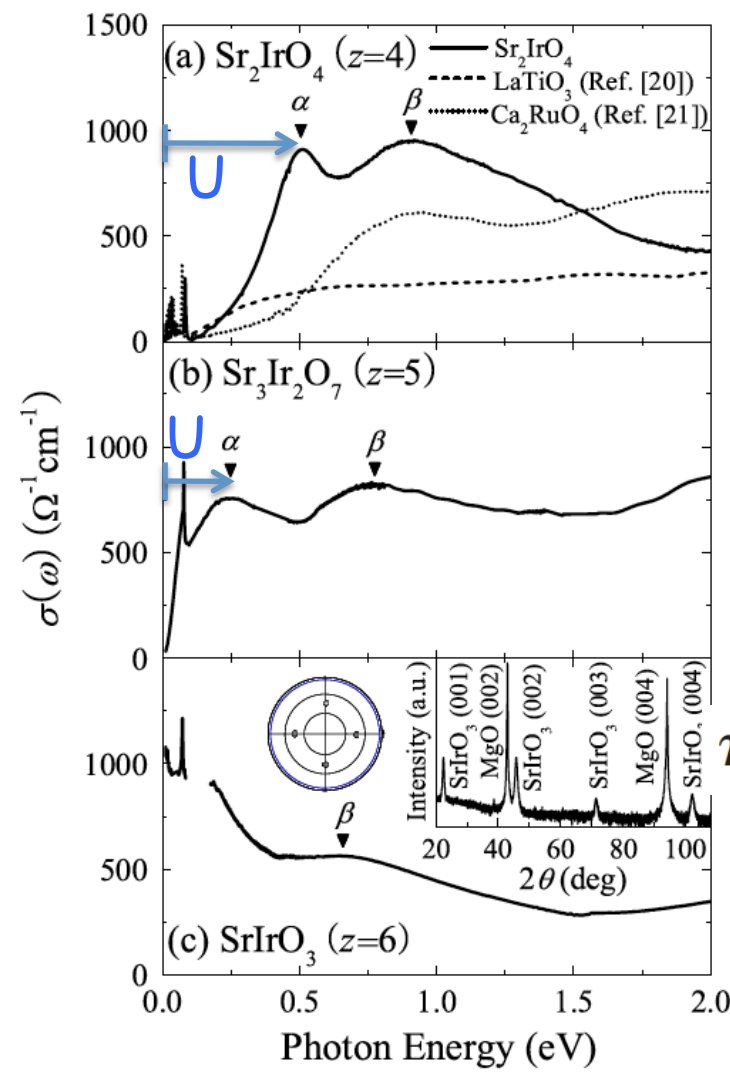


# Optical spectroscopy on RP iridates

n=1:  $\text{Sr}_2\text{IrO}_4$   
 $\Delta_c = 0.35 \text{ eV}$

n=2:  $\text{Sr}_3\text{Ir}_2\text{O}_7$   
 $\Delta_c$  very small  
(unresolved)

n= $\infty$ :  $\text{SrIrO}_3$   
metal



$$\eta = J_H / U$$

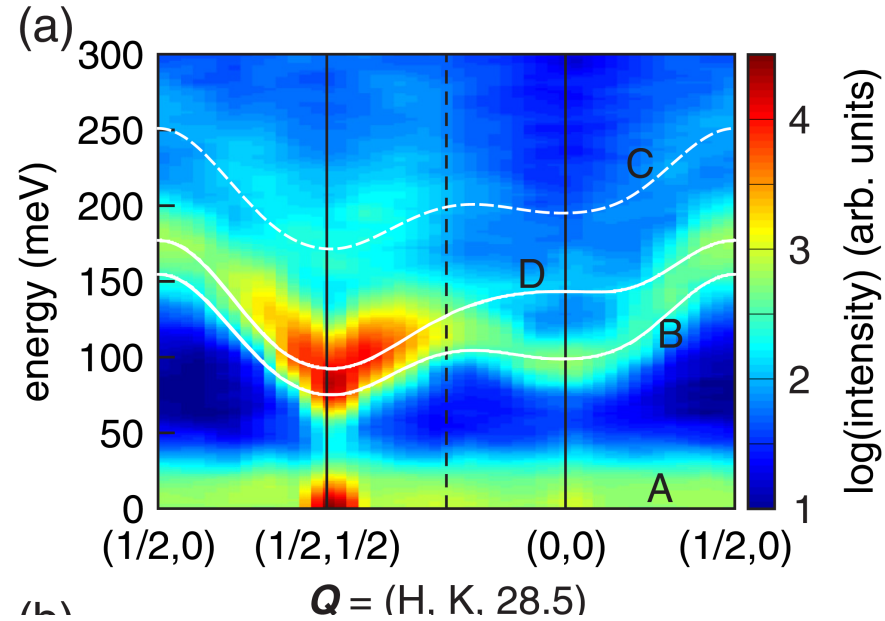
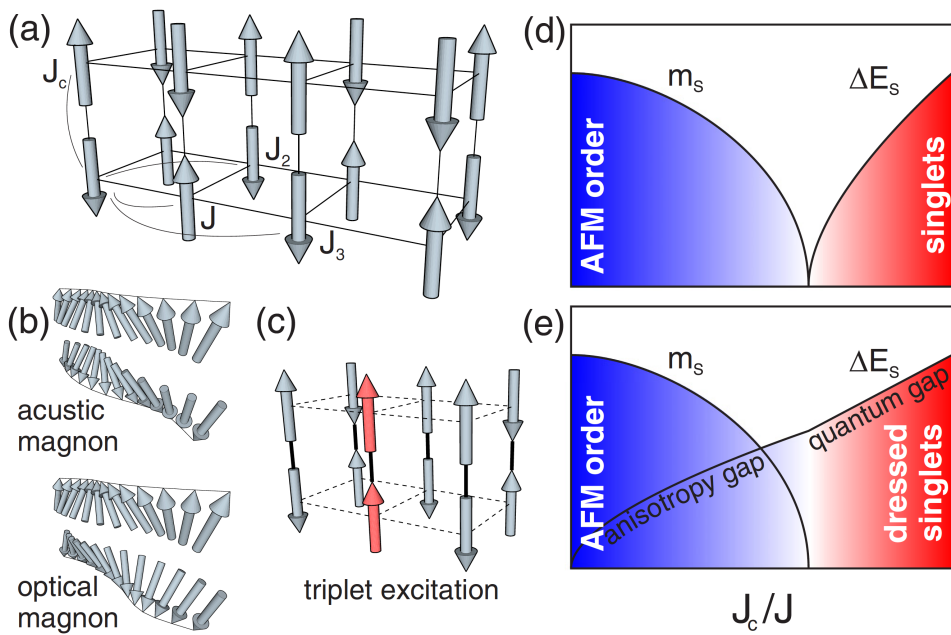
# Alternative model

PHYSICAL REVIEW B 92, 024405 (2015)

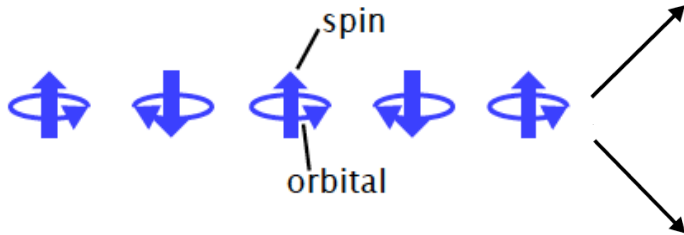
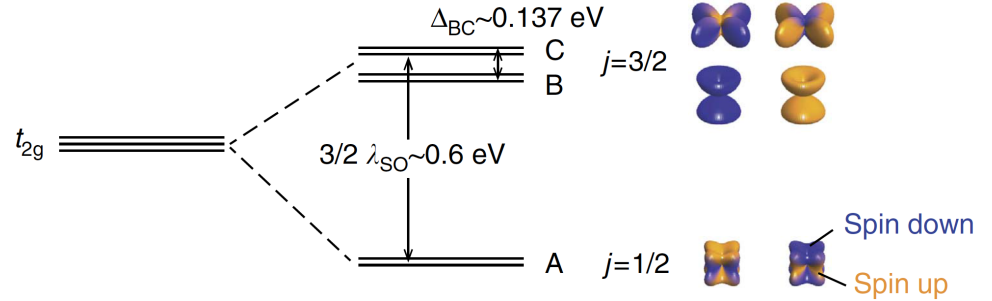
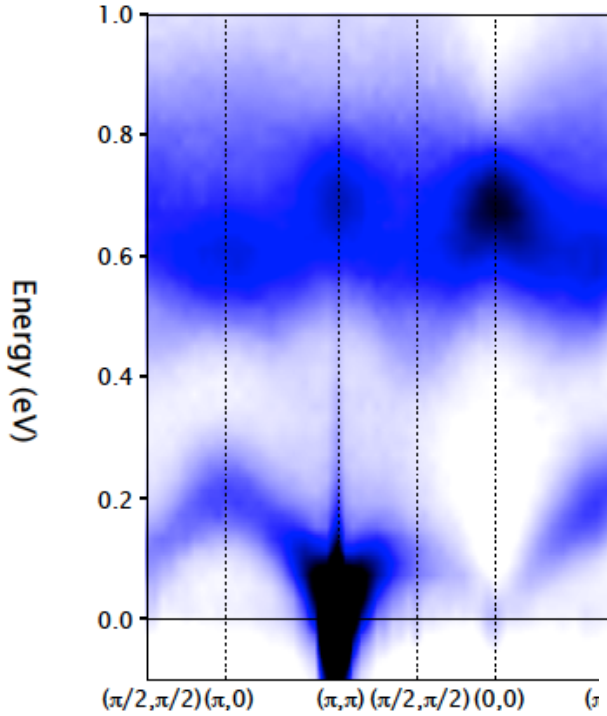
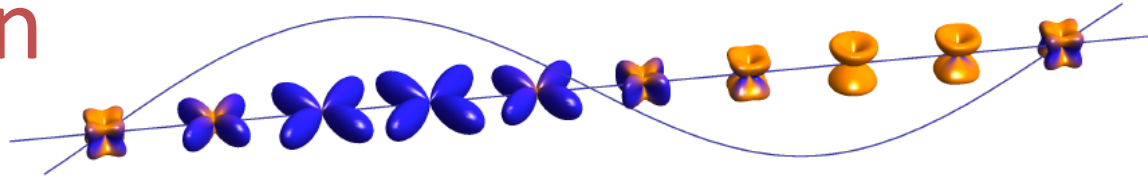


## Evidence of quantum dimer excitations in $\text{Sr}_3\text{Ir}_2\text{O}_7$

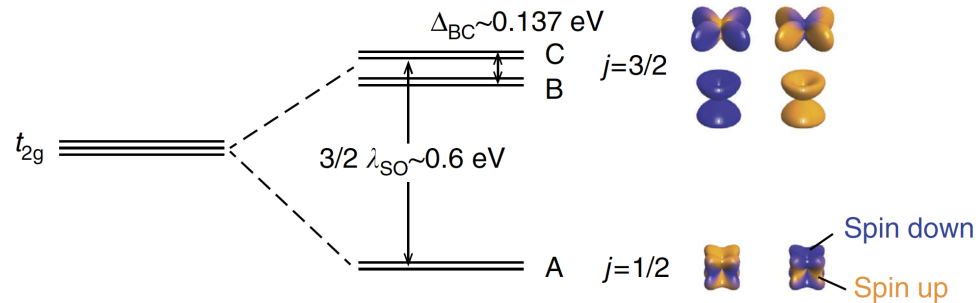
M. Moretti Sala,<sup>1</sup> V. Schnells,<sup>2</sup> S. Boseggia,<sup>3,4</sup> L. Simonelli,<sup>1,5</sup> A. Al-Zein,<sup>1</sup> J. G. Vale,<sup>3</sup> L. Paolasini,<sup>1</sup> E. C. Hunter,<sup>6</sup> R. S. Perry,<sup>3</sup> D. Prabhakaran,<sup>7</sup> A. T. Boothroyd,<sup>7</sup> M. Krisch,<sup>1</sup> G. Monaco,<sup>1,8</sup> H. M. Rønnow,<sup>9,10</sup> D. F. McMorrow,<sup>3</sup> and F. Mila<sup>11</sup>



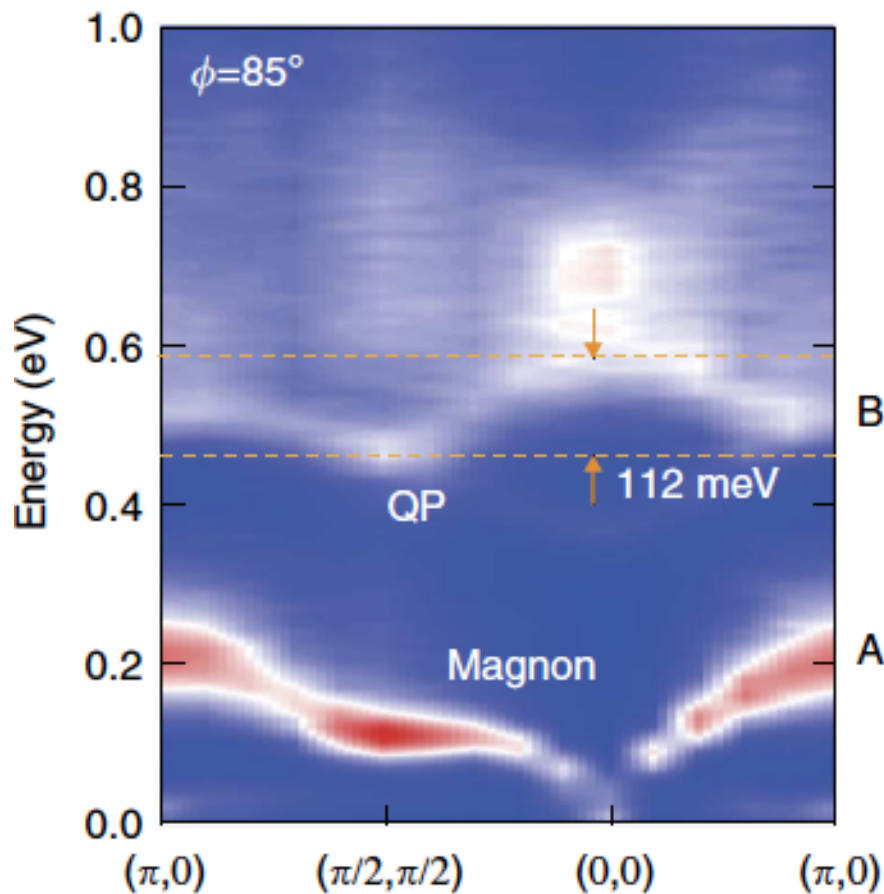
# Spin-orbit exciton



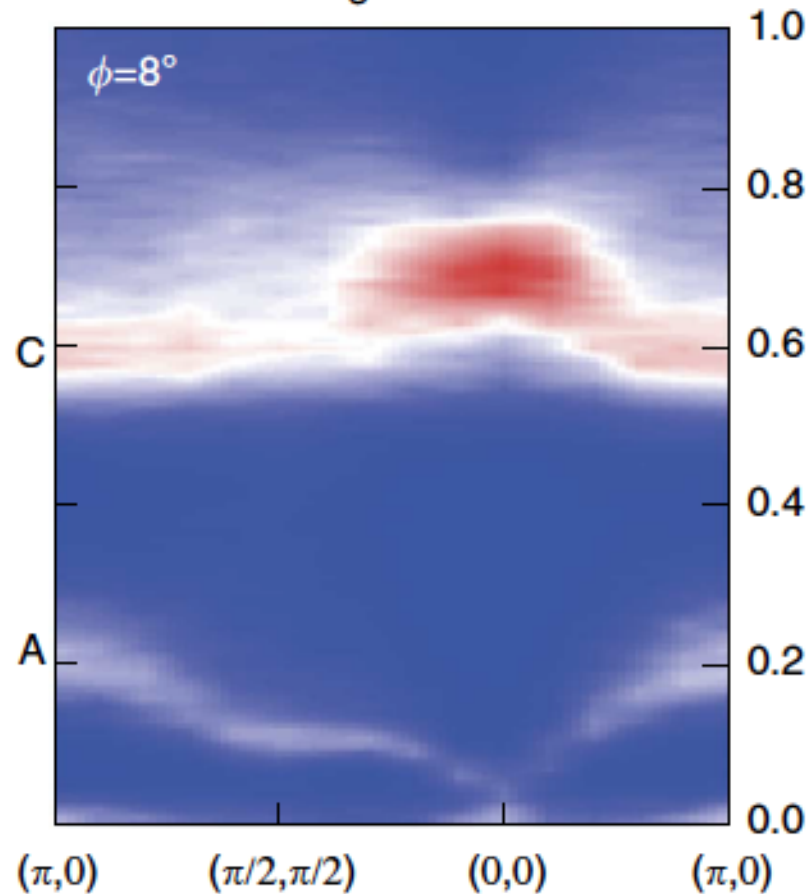
# Spin-orbit exciton



Normal incidence



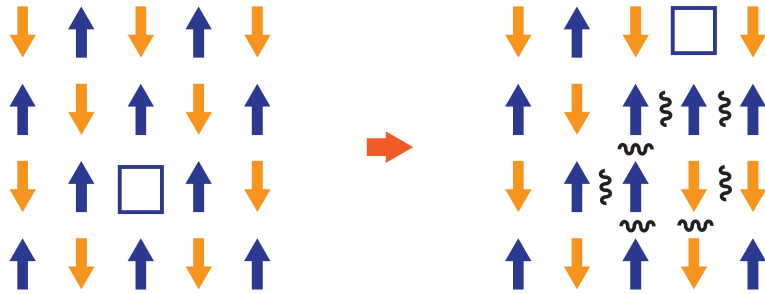
Grazing incidence



# One-hole problem


## ARPES (photon-in electron-out)



a hole propagation



initial

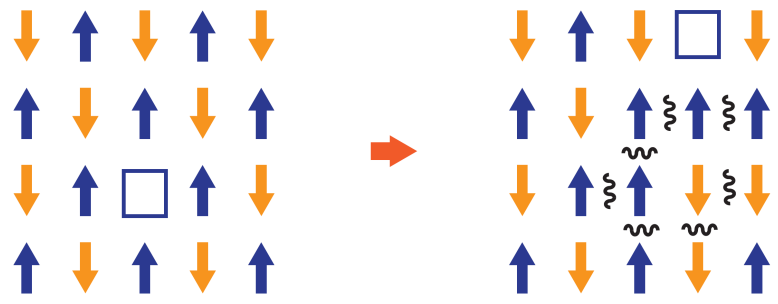
final

  
photon (+ vacuum)

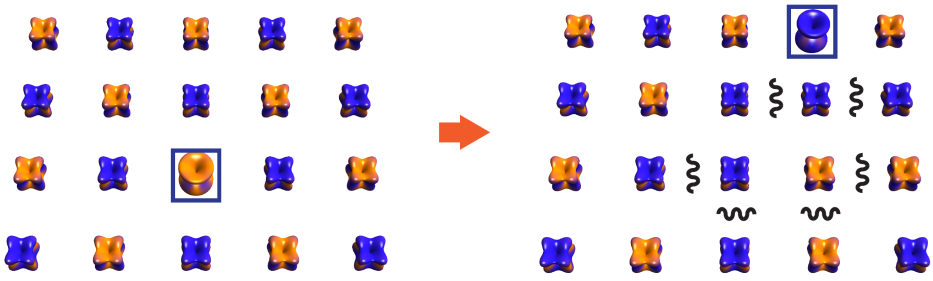
 photoelectron  
 hole left behind

# One-hole problem

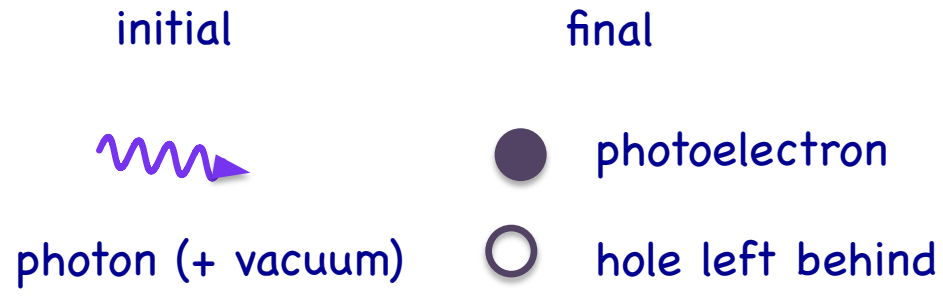
a hole propagation



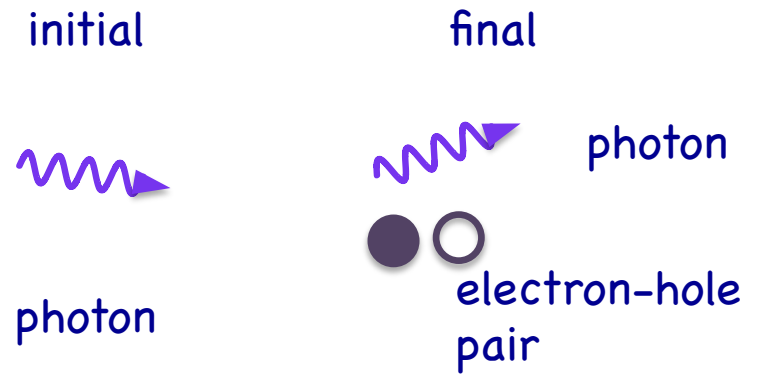
b exciton propagation



## ARPES (photon-in electron-out)



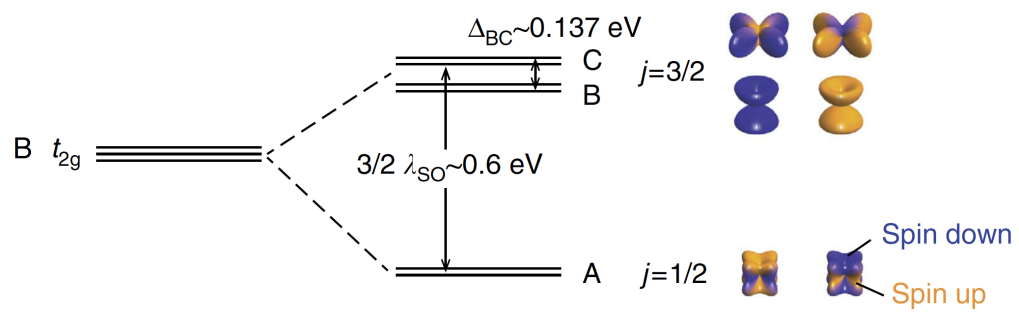
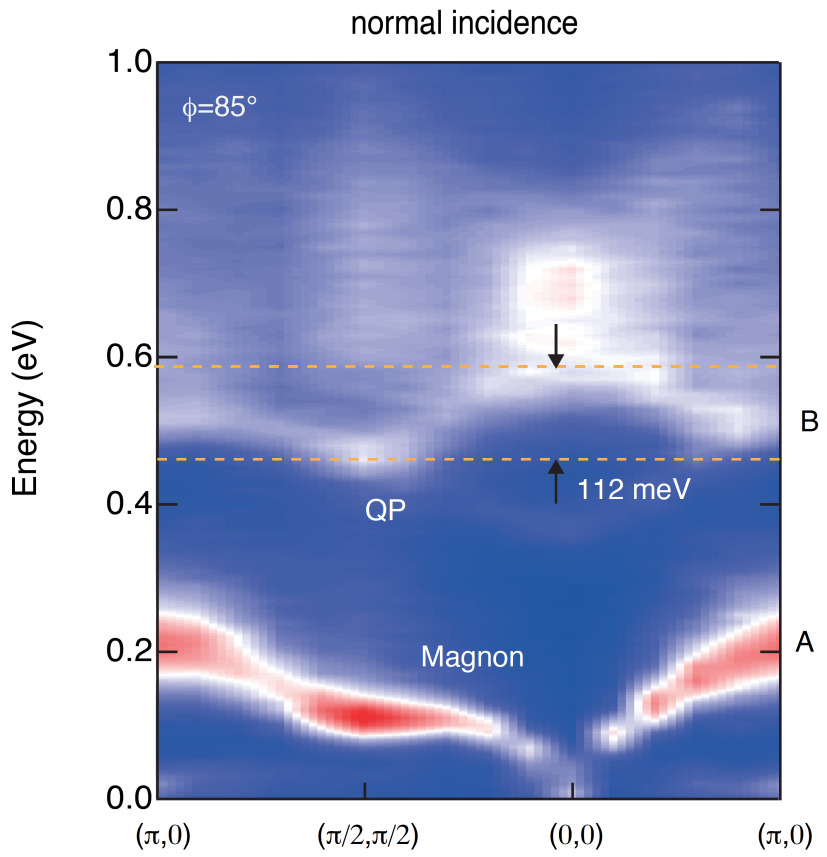
## RIXS (photon-in photon-out)





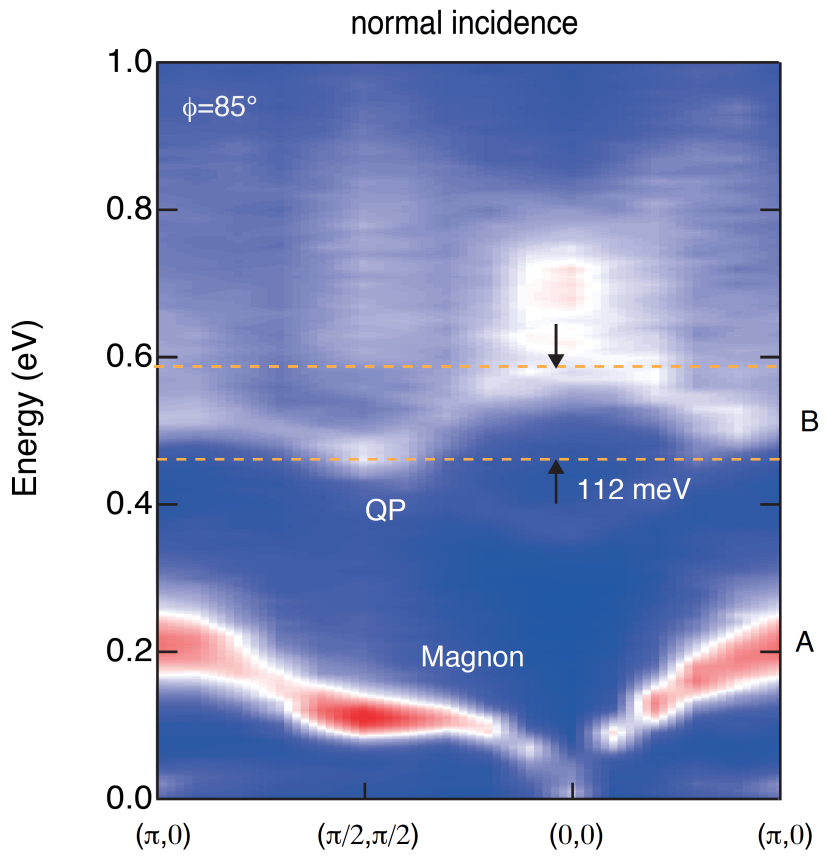
# One-hole problem

## a RIXS

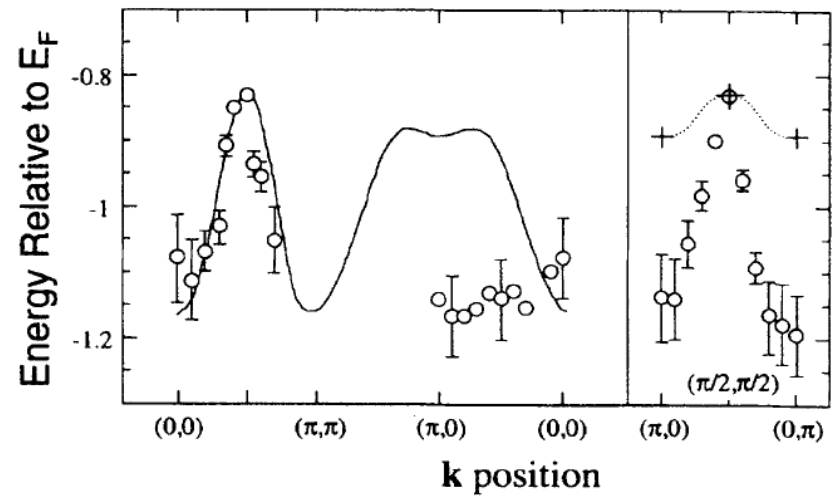


# One-hole problem

a RIXS

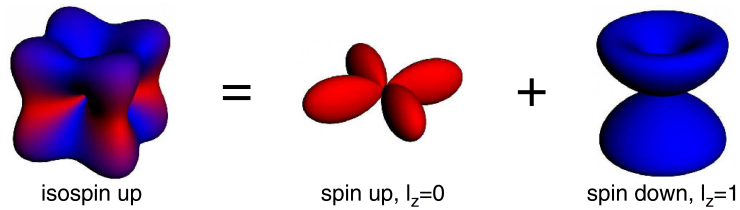


ARPES (cuprate)



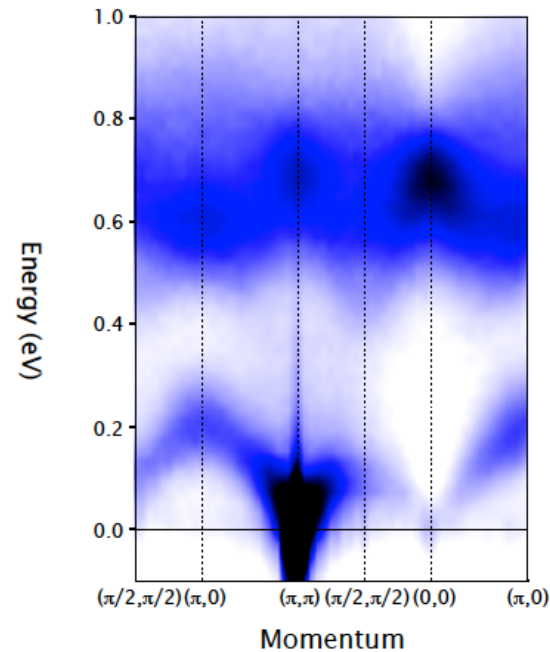
B. O. Wells et al., PRL (1995)

# Summary



RIXS is an excellent tool for 5d oxides to study magnetic excitations.

RIXD can not only solve the magnetic structure but also the spin-orbital structure



RIXS is sensitive to many other kinds of excitations beyond magnons

