Recent developments of model studies on molecular compounds

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Abstract:
To theoretically study molecular compounds, especially molecular (organic) conductors, we have successfully used effective models that take advantage of the relative simplicity of the electronic structure near the Fermi energy, despite their apparently complicated crystal structure [1]. Starting with an introduction to how such a scheme works, I will discuss two topics that we have recently been working on. 1) Theoretical proposals of novel spin transport properties (spin current conductivity [2] and anomalous Hall effect [3]) in antiferromagnetic phases: this idea has been applied to many materials and is now called "altermagnets". I will also briefly discuss inorganic perovskite compounds [4]. 2) Integration of first-principles calculation, effective model analysis, and experiments: Thanks to the development of computing power and applications, we can now derive effective models and evaluate their parameters at a qualitative level, providing feedback to experiments that was not possible before. I will present several examples, including a comprehensive analysis of classical quasi-one-dimensional materials based on the TMTTF/TMTSF molecules [5], and a yet-another evaluation of effective interactions in the quantum spin-liquid material based on Pd(dmit)2 molecules [6].

References:
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