Interpretable Machine Learning for Design of Novel Strongly Correlated Electron Materials

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Strongly correlated electron materials (SCEMs) possess various exotic properties including unconventional superconductivity in copper oxides and various magnetic phases in Heusler compounds. These can be harnessed for concrete applications, including lossless transportation of electricity at temperatures above the boiling point of nitrogen, memory devices with low power consumption using spintronics, and environmentally friendly magnetocaloric refrigeration.

To create new functional SCEMs, the first key point is to understand how these properties emerge from strong electronic correlations. This can be achieved using a combination of experimental and theoretical frameworks, including electron spectroscopy and *ab initio* calculations of the electronic structure, which have been widely used to study SCEMs.

The second key point is to understand how these properties vary with the material. This requires machine learning to analyze large sets of experimental or numerical data and to extract how macroscopic properties (e.g., the superconducting or magnetic transition temperature T_c) depend on microscopic electronic-structure descriptors such as hopping amplitudes, orbital character, and onsite magnetic moments, which are directly connected to spectroscopic observables. Interpretable machine learning is particularly useful in this context, as it yields explicit relations between T_c and low-energy Hamiltonian parameters or magnetic moments obtained from *ab initio* calculations, providing a direct bridge between electronic-structure theory, spectroscopy, and macroscopic properties.

In this talk, I will present recent developments of interpretable machine-learning procedures [1] and their application to copper oxide superconductors and collinear Heusler magnets [1,2]. These works reveal how superconducting or magnetic transition temperatures can be controlled by tuning the chemical formula, providing theory-guided guidelines for interpreting experimental trends and for the design of new functional SCEMs.

References

[1] J.-B. Morée and R. Arita, Phys. Rev. B **110**, 014502 (2024).

[2] J.-B. Morée, J. Bouaziz and R. Arita, arXiv:2510.18469 [cond-mat.mtrl-sci] (2025)