Theoretical design of correlated topological materials by integrating first principles simulation and spectroscopy

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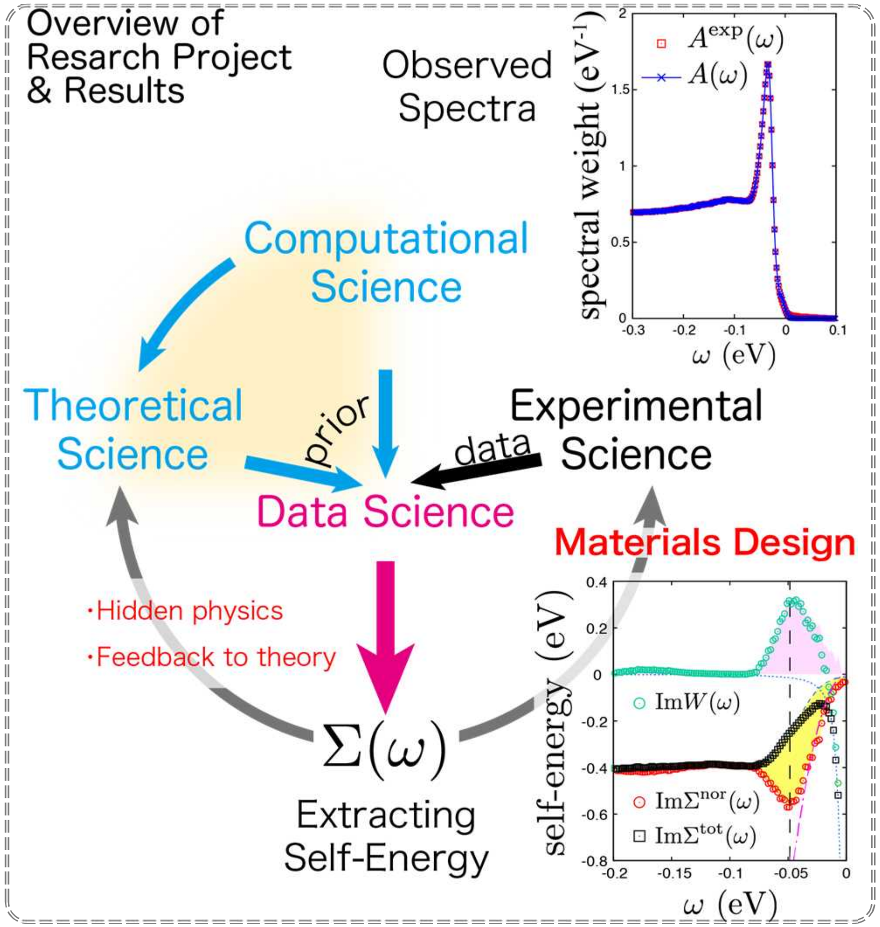
Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences (PO: Shinji Tsuneyuki)

Brief overview

Theoretical design of functional materials including high temperature superconductors and correlated topological materials is the goal of the research project. By integrating theoretical and computational approaches with experimental researches based on data science, we tried to extract self-energy that describes how electrons are interacting each other and scattered by impurities and defects in correlated electron systems, and, however, is hidden in existing experimental methods; Together with developing direct methods that simulate self-energy, self-energy is inferred from experimental data by solving non-linear inverse problems with machine learning technology.

Achievement

We utilized the Boltzmann machine to extract physical quantities hidden in experimental data combined with physically sound prior knowledge. The method is developed by analyzing and applied to the angle-resolved photoemission spectroscopy spectra of a typical cuprate copper oxide superconductors, $Bi_2Sr_2CaCu_2O_{8+\delta}$ with a superconducting transition temperature 90 K, to extract the metallic (normal) and superconducting (anomalous) contributions in the self-energy separately, in which mutual interactions among electrons are encoded. We found prominent peak structures emerging both in the normal and anomalous self-energies, which are canceled in the total self-energy and hence invisible in experiments, as the origin of high-temperature superconductivity (see the right figure). The present achievement may open avenues for innovative machine-learning spectroscopy of correlated topological materials.



Reference/Link

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Extraction of self-energy by machine learning: Y. Yamaji, T. Yoshida, A. Fujimori, and M. Imada (2019), submitted.
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As for related strategic objectives related to this research area, see http://www.senryaku.jst.go.jp/teian/en/koubo/h29youkou_7_en.pdf