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NCCR MARVEL Distinguished Lecture

Using the right criteria for design and discovery

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Abstract: Materials design and discovery require a thorough knowledge of the underlying physics. Incomplete understanding can lead to misguided searches, both experimentally and computationally. I will illustrate these points with two case studies.

The Mott-Hubbard gaps of rare-earth titanates are commonly reported to be 0.2-0.7 eV. These values are based on optical reflectivity measurements, from which the onset of optical absorption is derived. Rigorous computational and experimental studies for $GdTiO_3$ indicate that the gap is significantly larger, and that the previously identified feature in the optical absorption is due to the excitation of small hole polarons. These findings likely apply to a broader set of materials, and impact the design of complex-oxide heterostructures as well as the search for materials in which the metal-insulator transition can be exploited.

Defect-assisted nonradiative recombination can severely affect the efficiency of electronic and optoelectronic devices. The rule of thumb for assessing whether a defect will lead to strong nonradiative recombination has been based on whether the defect level is close to mid-gap. However, we have found that strong nonradiative recombination can occur for defects that fail to meet this criterion. These insights also impact the search for novel qubits or single photon emitters for quantum information science.

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