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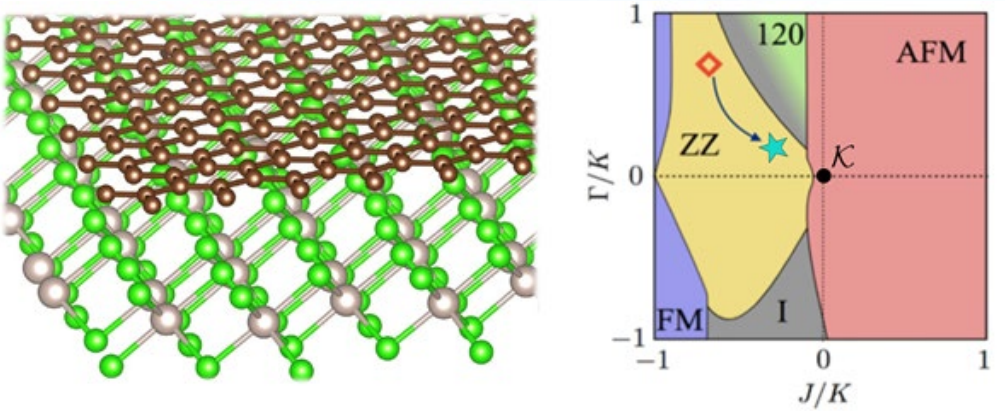
New theoretical approach to tackle interface quantum materials

E. Gerber, Y. Yao, T.A. Arias, and E-A. Kim Cornell

The Materials-by-Design approach relies on strong theoretical capabilities to predict the properties of novel materials. Unfortunately, traditional *ab initio* techniques for calculating the electronic structure of materials are powerless when the lattice mismatch between two crystals leads to the absence of periodicity, as observed between many of the interface quantum materials that are the focus of PARADIM's in-house research.

To overcome this issue, Kim and Arias developed Mismatched Interface Theory (MINT) to study such interfaces theoretically. Our first application of MINT is to the graphene/α-$RuCl_3$ hetero-bilayer interface enabling a quantitative prediction of charge transfer between the two monolayers.

MINT is based on a simple principle and it uses established and widely available standard *ab initio* methods in each of its steps. Hence MINT is versatile and accessible, and we anticipate the application of this approach to produce many more exciting results in mismatched interface systems previously out of reach of *ab initio* studies.



(left) The highly mismatched interface material formed by bringing a monolayer of graphene into contact with a monolayer of α-$RuCl_3$.
(right) The result (green star) of our *ab initio* MINT calculation for the graphene/α-$RuCl_3$ bilayer added to the Luttinger-Tisza phase diagram from Kim *et al. Phys. Rev. B* **91**, 241110 (2015). The red diamond represents the ground state of plain α-$RuCl_3$. Our MINT calculations indicate that the charge transfer from graphene to α-$RuCl_3$ brings this interface quantum material much closer to the Kitaev point ($\mathcal{K}$) at the origin, relevant to quantum computing applications.

DMR DIVISION OF MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

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