

Design of Layered Materials and Interfaces by First-principles Method



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Abstract

Two-dimensional materials has gained great attentions for implications in nanoelectronics and photonics. The optical and electronic properties of two-dimensional materials supported on copper-based superconductors is presented. Notably, when monolayer-WSe₂ is placed on La_{1.85}Sr_{0.15}CuO₄ (WSe₂/LSCO), it exhibits a distinctive band structure that sets it apart from monolayer-WSe₂ supported on other substrates. Through the application of high-resolution spectroscopic ellipsometry and density functional theory calculations, we have determined that this unique electronic structure can be attributed to the formation of an interfacial small polaron at the WSe₂/LSCO interface. This formation is driven by charge transfer between the CuO₂ plane of the cuprate superconductor and the WSe₂ layer. In addition, we present an efficient high-throughput screening high- κ dielectrics from a large materials database, of which 2D Sb₂S₂O₉, two Bi₂O₃ phases, As₂S₂O₉, Sb₂O₃, and Te₂H₂O₃F₄ have been predicted to be the most promising gate dielectrics due to their optimal trade-off between dielectric constant and band gap, as well as facile growth possibility.

Biography

Prof. Ming YANG is currently an Assistant Professor at Hong Kong Polytechnic University in Department of Applied Physics. He obtained his Bachelor at Fujian Normal University in 2001 and PhD at National University of Singapore in 2010. His recent research focuses on accelerating the development of functional materials using high-throughput screening techniques, large-scale DFT calculations, and machine learning. Prof. Yang also engaged in developing 2D electronic and spintronic devices, as well as exploring the electronic, magnetic, topological, and optical properties of 2D materials and their heterostructures. To date, Prof. Yang has published over 200 peer-reviewed papers in renowned journals such as Science, Nat. Mater., Nat. Electron., Nature Nanotech., PRL, Adv. Mater., and JACS. Prof. Yang's work has received more than 9000 citations, with an H-index of 50 (as of November 2025, Google Scholar). Additionally, Prof. Yang have contributed to two book chapters and filed three PCT patents.