Abstract Submitted
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First-Principles Modeling for Low-Energy Electron Diffraction Spectra[1] JOHN MCCLAIN, University of New Hampshire, JIEBING SUN, Michigan State University, JAMES HANNON, IBM Thomas J. Watson Research Center, KARSTEN POHL, JIAN-MING TANG, University of New Hampshire — We present a computational method to incorporate density-functional theory (DFT) into the calculation of the reflectivity in low-energy electron diffraction (LEED). Rapid and accurate analysis of diffraction spectra will facilitate the development of low-energy electron microscopy. The dynamical analysis of the electron reflectivity is traditionally carried out using multiple scattering theory with spherically symmetric (muffin-tin) potentials. However, for directionally bonded materials, such as semiconductors, the actual crystal potentials in the interstitial region can be significant, particularly for very low energy electrons. DFT with nonlocal pseudopotentials yields the low-energy electronic structure more accurately. In typical DFT calculations for surfaces, a finite slab is set up in a large unit cell with periodic boundary conditions. By matching the plane waves representing the LEED beams to the Kohn-Sham wave functions at the boundaries of the supercell, we determine the diffraction intensities. To demonstrate that our matching approach is not limited by the finite size of the supercell, we first consider trial models with exact solutions. We then use this approach to analyze the electron diffraction from graphene and compare with features in the band structure.

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