Abstract Submitted
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First-Principles Calculations of LEEM Reflectivity Spectra of Molybdenum Disulfide[1] JOHN MCCLAIN, Integrated Applied Mathematics, University of New Hampshire, KARSTEN POHL, Department of Physics and Materials Science Program, University of New Hampshire, JIAN-MING TANG, Department of Physics, University of New Hampshire — We present calculations of the low-energy electron specular reflectivity spectra of systems of a few layers of molybdenum disulfide at general angles of incidence using a newly modified algorithm within our first-principles theoretical approach, which leverages the self-consistent scattering potentials produced by density-functional theory [1]. Our calculated normal-incidence spectra for MoS_2 reveal layer-dependent features around 7-8 eV and 15 eV, allowing for a characterization of the number of layers via LEEM reflectivity and thus an in-situ technique for growth monitoring. We have previously described the application of our approach to the off-normal spectra of few-layer graphene, but the lack of mirror symmetry in MoS_2 requires a new algorithm for finding degenerate pairs of solutions for the matching procedure. The computed off-normal spectra illustrates the complexity of the electronic structure of MoS_2. We also present the way in which our new off-normal algorithm leads naturally to an approach to higher-order diffraction intensity calculations with the wave-matching scheme, along with our results for higher-order diffraction in model systems and progress towards results for real systems. [1] McClain et al., arXiv.1311.2917.

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