First-Principles Computation of Low-Energy Electron Diffraction Spectra of 2D Materials

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11:00 a.m.
SH 202
Coffee and refreshments 10:45 a.m. in SH 108

Low-energy electron diffraction (LEED) is an experimental tool that measures the intensity of low-energy electrons back-diffracted from crystalline surfaces. By varying the energy of the electron beam, a so-called LEED IV curve can be recorded. Comparing these experimental curves to curves calculated from models of the surface can reveal detailed information about the surface, like atomic spacing, layer spacing, and layer stacking. Conventional calculation methods use simplified atomic potentials and rely on empirically determined fitting parameters.

I will present our first-principles, computational method for modeling the diffraction of low-energy electrons from crystalline surfaces [1], showing calculated LEED IV curves for two examples of the exciting, new class of 2D materials, graphene and MoS_2. First, I will give a brief overview of electronic structure calculation in solid state physics, including the natural way in which Fourier methods arise, Bloch's Theorem, band structures, and density-functional theory (DFT). Then, I will explain how we have developed a straight-forward 'boundary matching,' Fourier method for solving the Schrödinger Equation in a scattering geometry that allows for the incorporation of the realistic potentials that DFT can provide. I will show our results as compared to experiment and discuss avenues for improvement. Finally, time permitting, I will discuss some numerical issues with solving the Schrödinger Equation in this setting, and two methods for handling them, namely the Numerov method and Singular Value Decomposition. This is joint work with Drs. Jian-Ming Tang and Karsten Pohl. [1] McClain *et al.*, arXiv.1311.2917.

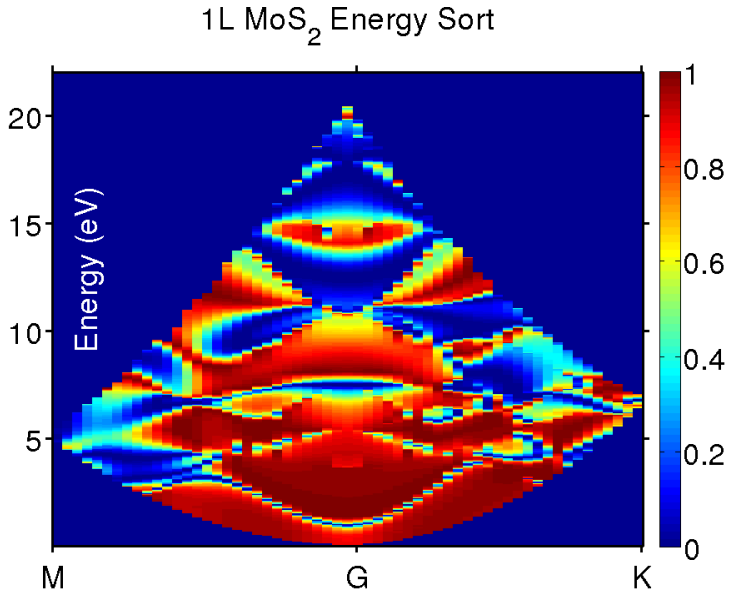

Figure 1: Off-Normal Reflectivity Spectra for One Layer MoS_2

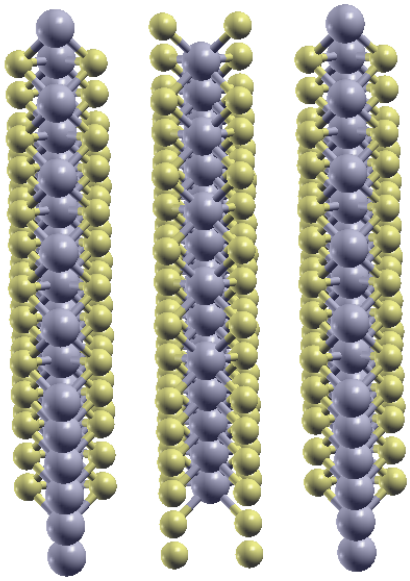

Figure 2: Structure of Three-Layer MoS_2