Modeling the interaction of two-dimensional materials with moving charged particles

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This talk reviews several recent results achieved with collaborators in the mathematical modeling of two-dimensional (2D) materials within the context of electron microscopy and similar probes. Using graphene and phosphorene as prototypes of isotropic and anisotropic 2D materials, respectively, the electron energy loss spectra (EELS) and related quantities—such as the stopping force on a moving charge and the induced wake potential—are examined. Using suitable models for the in-plane response of 2D materials, the focus is placed on the signatures of plasmon mode excitation by an incident charged particle, as well as their hybridization with phonon modes in the dielectric environment. While select results for graphene are compared with available experimental EELS data, several consequences of the anisotropic in-plane response of phosphorene are discussed, including the application of the Energy Loss Method to compute its electrical DC conductivity tensor. Finally, the effects of the out-of-plane response of 2D materials are analyzed using generalized boundary conditions for Maxwell's equations that treat these materials as polarizable sheets of zero thickness.