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Multiscale modeling of nanostructures for electronic and energy-related applications

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The optimization of materials properties for opto-electronic and energy-related applications is a crucial component in the design of new devices. To this end, multiscale modeling of nanostructures is essential in understanding and predicting materials properties ranging from optical response to the mechanical failure. We present a number of examples where multiscale modeling has yielded useful information concerning the optimal choices for nanostructured device elements. These include the excitation and charge transfer processes in hybrid photovoltaic devices, the tuning of optical and electrical properties of layered materials like graphene and transition-metal-dichalcogenides, and the mechanical response and deformation of silicon-based high-energy-density electrodes.