# Electronic and Optical Properties of Ultrathin Materials from First Principles

**Emmanouil Kioupakis**

*Materials Science and Engineering, University of Michigan*
kioup@umich.edu

We use first-principles calculations based on density functional and many-body perturbation theory to analyze the effects of quantum confinement on the band gap, excitons, and optical properties of two-dimensional materials, as well as ultrathin nitride nanowires and quantum wells. Our calculations for single-layer and double-layer SnSe and GeSe show that these materials exhibit an unusually high absorbance (approaching 40-50%) in the visible range and that they are promising for ultrathin photovoltaic applications. Moreover, our results for few-layer PbI2 reveal the intermediate nature of excitons between the Wannier and Frenkel picture in this material [1]. We also examined the optical properties of ultrathin InN nanowires and GaN quantum wells. Our results show that InN nanostructures with a dimension of ~1 nm can be applied for efficient green-light emission [2], while ultrathin GaN quantum wells with a thickness of 1-4 monolayers can be used for deep ultraviolet LEDs for germicidal applications.

[1] A. S. Toulouse, B. P. Isaacoff, G. Shi, M. Matuchov, E. Kioupakis, and R. Merlin, Phys. Rev. B 91, 165308 (2015).

[2] D. Bayerl and E. Kioupakis, Nano Lett. 14, 3709–3714 (2014).