Ions on the verge of ionization¹ VAZGEN SHEKOYAN, Rutgers University, Department of Physics and Astronomy, KIERON BURKE, Rutgers University, Department of Chemistry and Chemical Biology — The behavior of negative ions on the verge of ionization is studied. Electron-electron correlation plays a significant role for negative ions, especially for the outermost electron. Answering questions such as what negative ions exist, what the behavior of its electronic density is at the ionization threshold or why negative ions are particularly hard to treat in Density Functional Theory (DFT) are important. A general formalism (a differential equation for the square root of the electronic density) has been developed to treat such systems. It has been applied on a 1-d model of 2-electron negative ion, and its behavior on the verge of ionization has been studied in detail.

¹This work is supported by NSF/CHE-0355405.

Vazgen Shekoyan
Rutgers University, Department of Physics and Astronomy