Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A first-principles study of weakly bound molecules using exact exchange and the Random Phase Approximation[1] HUY-VIET NGUYEN, GIULIA GALLI, University of California, Davis — We present a study of the binding energy (BE) curves of rare gas and alkaline-earth dimers using an energy functional that includes exact exchange (EXX), and correlation energies within RPA. Our results for the equilibrium positions, and long range behavior of the potential energy curves show great improvements over those obtained at the standard LDA/GGA DFT levels. For Ar and Kr, our BE results are improved as well and are comparable to that of so-called vdW-DF functional, although EXX/RPA yields BE curves that agree better with experiment for large separation distances, as expected. We also discuss shortcoming of the EXX/RPA perturbative approach and analyze possible sources of error in the description of the BE curve of alkaline-earth dimers, in particular Be_2, exhibiting an unphysical maximum at large separation. We suggest that the lack of self-consistency in current EXX/RPA approaches might be largely responsible for most of the observed shortcomings. Finally we present a tight binding approach to obtain the eigenvalues of the dielectric matrix entering the calculation of the RPA correlation energy, that greatly improves the efficiency of EXX/RPA calculations.

[1]Work supported by DOE/Scidac grant DE-FC02-06ER25794 and DOE/BES grant DE-FG02-06ER46262.

Huy-Viet Nguyen
University of California, Davis

Date submitted: 17 Nov 2009 Electronic form version 1.4