Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecules Without Atoms[1] ANTHONY RUTH, LAURA COLLINS, KENJIRO GOMES, BOLDIZSAR JANKO, Univ of Notre Dame — We present a real-space representation of molecules which results in the normal bonding rules and electronic structure of chemistry without atom-centered coulomb potentials. Using a simple mapping, we can generate atomless molecules from the structure of real molecules. Additionally, molecules without atoms show similar covalent bonding energies and transfer of charge in ionic bonds as real molecules. The atomless molecules contain only the valence and conduction electronic structure of the real molecule. Using the framework of the Atoms in Molecules (AIM) theory of Bader, we prove that the topological features of the valence charge distribution of molecules without atoms are identical to that of real molecules. In particular, the charge basins of atomless molecules show identical location and quantities of representative charge. We compare the accuracy, computational cost, and intuition gained from electronic structure calculations of molecules without atoms with the use of pseudopotentials to represent atomic cores in density functional theory.

[1]A. R. acknowledges support from a NASA Space Technology Research Fellowship

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Date submitted: 11 Nov 2016 Electronic form version 1.4