Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Inverse Molecular Design in a Tight-Binding Framework DEQUAN XIAO, WEITAO YANG, Department of Chemistry, Duke University, Durham, NC 27708, DAVID BERATAN, Department of Chemistry and Department of Biochemistry, Duke University, Durham, NC 27708 — The number of chemical species of modest molecular weight that can be accessed with known synthetic methods is astronomical. An open challenge is to explore this space in a manner that will enable the discovery of molecular species and materials that exhibit optimized properties. Recently, a strategy was developed to perform continuous optimization of molecular properties, the linear combination of atomic potentials (LCAP) approach.[1] Here, using a simple tight-binding (TB) implementation, we show that the LCAP strategy can successfully explore vast chemical libraries that are based on planar π-electron motifs. We show that LCAP property optimization of π-electron polarizabilities and hyperpolarizabilities is effective for libraries with 10^4 to 10^{16} members. This approach finds optimal structures among 10^4 candidates with about 40 individual molecular property calculations. As such, for molecular candidates with strong structural similarity, the TB-LCAP approach may provide an effective means of identifying structures with optimal properties.

[1]M. Wang, X. Hu, D. N. Beratan, and W. Yang, J. Am. Chem. Soc. **128**, 3228 (2006); S. Keinan, X. Hu, D. N. Beratan, and W. Yang, J. Phys. Chem. A **111**, 176 (2007).

Dequan Xiao
Department of Chemistry, Duke University, Durham, NC 27708

Date submitted: 23 Nov 2007 Electronic form version 1.4