Rational Organic Semiconductors Materials Design One Screensaver at a Time

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There is a wide interest in finding new high performance, air-stable organic semiconductors for their use in a number of electronic devices, such as field effect transistors, light emitting diodes, and solar cells. Motivated by recent experimental results on naphtho[2,3-b]naphtho[2',3':4,5]thieno[2,3-d]thiophene, which has demonstrated stability under ambient conditions and a relatively high (2-3 cm^2/Vs) hole mobility, we have computationally explored the charge-transport properties of a number of related chemical compounds using a combination of density functional theory and molecular mechanics simulations. After validating our approach against known experimental and theoretical results, we predict that anthra[2,3-b]anthra[2',3':4,5]thieno[2,3-d]thiophene and pyreno[1,2-b]pyreno[2',1':4,5]thieno[2,3-d]thiophene will have remarkably high hole mobilities, 9.8 and 3.2 cm^2/Vs, respectively. In a similar spirit, towards the end of 2008, we developed a screensaver (http://cleanenergy.harvard.edu) together with IBM, which allows individual users anywhere in the world to contribute their idle computer time to perform computational chemistry calculations on combinatorial molecular libraries derived from fused aromatic molecules. Our objective is to aid the rational design of new π-conjugated materials suitable for organic electronics applications. The deployment of such a world-wide distributed computational engine has not been previously applied to atomic-scale modeling problems in material sciences, and therefore, it opens the doors for breakthroughs in the search of molecular materials for the next generation of organic semiconductors. Our theoretical calculations of the derivatives of [:4,5]thieno[2,3-d]thiophene along with the preliminary results of our combinatorial approach on organic molecular materials will be introduced at the conference.