475h Structure and Electronic Properties of Acene-Functionalized Polyhedral Oligomeric Silsesquioxanes (Poss) Molecules

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Atomistic computations, including ab initio quantum mechanics calculations and molecular dynamics (MD) simulations were performed to study a series of acene functionalized polyhedral oligomeric silsesquioxanes (POSS) molecules. First, the electronic properties of these novel molecules were determined using ab initio calculations. Then the structures that molecules with interesting electronic properties assemble into were predicted using Monte Carlo and MD simulations based on a classical force field. These structures were characterized in terms of their electronic, thermal, and mechanical properties. Our simulations reveal that the acene functionalized POSS configurations have similar band gaps than pure acene molecules, but have superior thermal and mechanical bulk properties. Moreover, the stacking of acene groups provides for increased pi-orbital overlap, and thus, electronic conductivity. Hence, these novel acene-functionalized POSS oligomers are potential new candidates for semiconducting organic/inorganic hybrid molecular materials, which have broad electronic applications. Our calculations contribute to the design and synthesis of new materials based on a nano building block self-assembly approach.