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Quantum molecular dynamics simulations of the stability and reactivity of aluminum cyclopentadienyl clusters SUFIAN ALNEMRAT, JOSEPH HOOPER, Naval Postgraduate School — We report *ab initio* quantum molecular dynamics simulations of the thermal stability and oxidation of aluminum-cyclopentadienyl clusters currently being considered as novel fuels or energetic materials. These clusters contain a small aluminum core surrounded by a single organic ligand layer. The aromatic cyclopentadienyl ligands form a very strong bond with surface Al atoms, giving rise to a stable organometallic cluster which crystallizes into a low-symmetry solid-state material. Our calculated heat of combustion per unit volume of this solid is quite high (60% that of pure aluminum) with reaction kinetics potentially much faster than nanoscale metals. Though this compound can be experimentally produced in small quantities, it is quite volatile. Here we report theoretical studies of the stability and decomposition of these passivated aluminum clusters in the presence of oxygen using Car-Parrinello molecular dynamics. We also consider alternate ligand forms which offer significantly increased steric protection or contain groups (such as fluorine) which may react with the metallic core.

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