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A critical assessment of thiolate self-assembled monolayers (SAMs) on platinum.[1] YENNY CARDONA QUINTERO, HONG ZHU, RAMPI RAMPRASAD, University of Connecticut — Thiolate SAMs have been successfully anchored on metal surfaces, but a critical assessment of the impact on the structural and electronic properties of the metal surfaces has remained elusive. CH_3S and CF_3S were selected as model systems in this work, because of their simple structures which can provide insights about how the composition and electronegativity of SAMs affect the properties of metal-SAM systems. Density functional theory calculations have been used in this work to study the adsorption of CH_3S and CF_3S molecules on the Pt (111) surface at different coverage (1/3, 1/4, 1/6, 1/9 and 1/12) and adsorption sites (fcc and hcp). The geometry, adsorption energy and the work function of the Pt-SAM systems have been determined. Several interesting observations could be made: (1) the optimized SAM is tilted with respect to the Pt surface and the tilted angle decreases with the molecular coverage on the Pt surface; (2) the adsorption energy of both systems are almost always lower at the fcc site compared to the hcp one and shows a coverage-dependence; (3) the work function of Pt-SAM also shows a dependence on coverage and hence controlling the molecular coverage is probably an effective technique to tune the work function.

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