Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111)

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The interaction of thiol and thiolate containing molecules with gold (S-Au) has gained increasing interest because of its applications in molecular electronic devices and catalysis. In this context, the enhanced conductivity of thiophenol compared to alkanethiol represents an opportunity to develop more sensitive and selective gold-based devices by incorporating molecules with the aryl-thiol moiety into their structures. As has been proposed earlier, the thiol moiety is deprotonated after binding to gold, hence, we present here a comparative study of the S-Au bond strength between several neutral and deprotonated aromatic-sulfur systems in their anionic and radical forms with a detailed description of the nature of this interaction. The study was performed by means of computational chemistry methods, using a cluster of 42 Au atoms as a model of the Au(111) surface that allowed us to provide new chemical insights to control the S-Au interface interaction strength. Our results revealed t