Adsorption of azulene and naphthalene on coinage metal surfaces: insights from first-principles calculations

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Azulene and naphthalene have the same molecular formula ($C_{10}H_8$) but different motifs and different electronic properties. Naphthalene has a regular 6-6 motif, with two hexagons, while azulene has a pentagon and a heptagon (5-7 motif). The non-alternant topology of azulene and the absence of mirror-related molecular orbitals lead to significant differences in its electronic structure when compared to naphthalene; in particular, azulene exhibits non-uniform charge distribution, more localized frontier orbitals, large in-plane dipole moment and blue color. Here, we present a first-principles study of the adsorption of these isomers on the Ag(111) and Cu(111) surfaces. We show that azulene interacts more strongly with the metal surfaces than naphthalene. On Cu(111), in particular, azulene presents a significantly larger adsorption energy (by a factor of 2) and larger deformation than naphthalene; analyses of the density of states show that the molecular features of azulene completely disappear upon adsorption on Cu(111), indicating a chemisorption process. We will compare our results with data obtained from NIXSW and TPD measurements.