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Potential energy landscape of monolayer-surface systems governed by repulsive lateral interactions: the case of (3×3)**-I-Pt(111)** ALEXANDRE TKATCHENKO, NIKOLA BATINA, MARCELO GALVAN, Universidad Autonoma Metropolitana — Combined Density Functional Theory (DFT) and Monte Carlo (MC) approach is applied to study the potential energy landscape of four iodine atoms adsorbed on the Pt(111) surface in (3×3) unit cell. Three critical points were identified: (3×3)-sym and (3×3)-asym, corresponding to structures well-known from experimental studies, while the third one (3×3)-zigzag is a new structure not reported before. An interaction model fitted to DFT calculations allows us to explain the difference between arrangements of iodine monolayer in vacuum, air and solution environments as a result of different repulsion regimes.

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