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Structural investigation of pentacene on Ag(111) by density functional theory FATIH DANISMAN, Middle East Technical University, ERSEN METE, Balikesir University, SINASI ELLIALTIOGLU, Middle East Technical University — We have used density functional theory (DFT) calculations based on the projector augmented wave (PAW) method to investigate the initial growth patterns of pentacene ($C_{22}H_{14}$) on Ag(111) surface. Here we will report our initial findings and provide a discussion of the results from the point of view of our previous experimental findings. Pentacene prefers to stay planar on Ag(111) surface and aligns perfectly along lattice vector (1,-1,0) without any molecular deformation at a height of 3.74 Å. At 1 ML coverage the separation between the molecular layer and the surface plane extends to 4.14 Å due to intermolecular interactions weakening surface-pentacene attraction. While the first ML remains flat, the molecules on a second full pentacene layer rearrange in a herringbone fashion which is energetically slightly more preferable when compared with a second layer composed of flat lying molecules. With addition of third and fourth layers pentacene molecules continue to maintain the herringbone configuration, with the stability of the herringbone configuration relative to the flat one increasing to 0.13 eV for the 3 ML film, while the first ML always remains flat. Therefore, our calculations indicate bulk-like initial stages for the growth pattern.

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