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Pentacene Molecules on Inert Surfaces YINA MO, Department of Physics, Harvard University, PAUL MARAGAKIS, Department of Chemistry, Harvard University, EFTHIMIOS KAXIRAS, Department of Physics and Division of Engineering and Applied Sciences — We study the energetics and dynamics of pentacene molecules in vacuum and saturated diamond (111) surface and silica surfaces. Force field molecular dynamics simulations are applied to capture the van de Waals type interactions among the pentacene molecules and the substrates. The herringbone arrangement of the molecules is found to be optimal both in vacuum and on various inert surfaces. A 90 degree rotation of the entire structure relative to that experimentally reported is identified on the silica surfaces.

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