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Atomic structures and electronic properties of poly(3-hexyl thiophene) on ZnO(110-1) surface. SEFA DAG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The atomic structures of adsorbed poly(3-hexyl thiophene) (P3HT) polymers on the non-polar ZnO surface (110-1) are studied with molecular dynamics using ab initio adjusted atomic force fields, and the electronic structures of the resulting systems arc studied with direct ab initio calculations. We investigated different P3HT attachment orientations on the ZnO surface. We also studied the influence of the crystallization among the P3HT polymers to the polymer - ZnO attachment. We found that the strength of the attachment depends strongly on the P3HT crystal orientation, and to the partial charge of the surface Zn, O atoms and the end atoms of the P3HT. We studied the temperature dependence of the attachment, and the effects of the details of the attachment atomic structures to the electronic properties of the interface.

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