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Molecular Modelling of the OPV Active Material at the Vicinity of Ag Nanoparticles

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Abstract: Silver nanoparticles are used in the active layer of OPVs in order to increase performance. However little is known about their effect on the structure of the active materials. Using classical force fields and molecular dynamics simulations we studied the structural and energetic properties for PCBM and 3-hexyl-thiophene oligomers in the vicinity of fcc (111) silver nanoparticles surfaces. During this study we have developed a new set of parameters for Ag-organic interface interactions and we have adjusted appropriately the torsion parameters for the 3-hexyl-thiophenes. Through the simulations performed we have observed a preferred position for PCBM with the tail away from the Ag surface. Furthermore examining the adsorption energy, of the preferred PCBM positioning, at different temperatures and comparing to 3HT oligomers layers, lying flat on the Ag surface, we have discovered that while at temperatures below 100K the 3HT oligomers are the preferred phase to be adsorbed, while at higher temperatures the trend changes with the 3HT phase being less preferred to be adsorbed onto the surface.