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First Principle Study on Interaction of ZnO Nanoribbon and Polyethylene Glycol

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A density functional theory based first principle study is performed to understand the mechanism of interaction of ZnO molecules with a capping agent PEG. It is divided into three steps; first step is the optimization of single PEG chain, ZnO nanoribbon (ZNR) and PEG chain with ZNR. The structural analysis is a second step, where noticeable structural change is observed in ZNR in presence of PEG chain. In final step, the electronic structure study is performed and corresponding DOS, PDOS and band-gap are compared. A computational program SIESTA is used under density functional environment. This novel approach provides wide opportunities in photovoltaic applications.