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Abstract:

The sensing propensities of acetone molecule towards zinc oxide monolayers (ZnO-ML) have been studied by means of density functional theory (DFT) calculations. Our van der Waals induced first principles calculations revealed that pristine ZnO-ML barely binds acetone, which limits its application as acetone sensing materials. However the formation of vacancies and foreign element doping improves acetone binding drastically. Among several defects, divacancy, and metal doping Li, Sc and Ti functionalization on ZnO-ML has been found the most promising ones. Presence of dangling electrons and partial positive charges in case of vacancy-induced and metallized ZnO-ML respectively, is believed to enhance the binding of acetone on the monolayers. The acetone-ZnO binding behavior has been further explained through studying the electronic properties by density of states and charge transfer mechanism

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