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Pd-assisted hydrogen spillover on graphene and carbonnanotubes

SA LI, PURU JENA, Virginia Commonwealth University, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — Addition of a small amount of Pd precursors on carbon nanotubes has recently been found to substantially improve the hydrogen uptake. In spite of several attempts, a fundamental understanding of how the catalyst works has remained unattainable. Using first principles methods we have investigated hydrogen spillover on Pd-doped graphene and (8,8) carbon nanotube. Through molecular dynamics (MD) simulations, we found that each Pd can bind to three pairs of hydrogen molecules on graphene and only one pair of hydrogen molecule on (8,8) nanotube at 300K. This difference is attributed to the effect of curvature. The hydrogen molecules were found to dissociate and bind to carbon surface once the Pd atom is saturated with hydrogen. These results provide important new insight to understand hydrogen spillover on carbon based materials.

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