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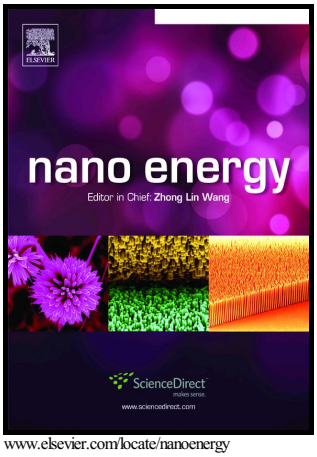

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Humidity-dependent piezopotential properties of zinc oxide nanowires: Insights from atomic-scale modelling

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Abstract

The humidity effect is inevitable in the fabrication and operation of zinc oxide (ZnO) nanowires (NWs). In this paper, the piezopotential properties of ZnO NWs under the humidity condition are compressively investigated based on atomic-scale simulations. Through molecular dynamics simulations, we find a mixed molecular and dissociative adsorption of water on the surface of ZnO NWs under the humidity condition. Absorptions of molecular and dissociative water both structurally reconstruct the surface atoms of ZnO NWs and thus modify their surface properties, which finally make the material properties of ZnO NWs under the humidity condition significantly different from those of their counterparts under the vacuum condition. Applying the obtained material properties to the numerical and analytical calculations of the piezopotential of ZnO NWs, we find a significant reduction in the piezopotential induced by the humidity effect. Similar to the results observed in the previous experiments, the reduction in the piezopotential is found to become more significant as the humidity level increases, since in this process more surface atoms of ZnO NWs will be adsorbed by molecular or dissociated water. Moreover, our density functional theory calculations indicate that the humidity effect can also influence the semiconducting properties of ZnO NWs by downward shifting their conduction band edges. However, the change in semiconducting properties induced by the humidity effect is found to have trivial effect on the piezopotential of ZnO NWs.

Keywords: Zinc oxide nanowire; Piezotronic; Piezopotential; Humidity effect