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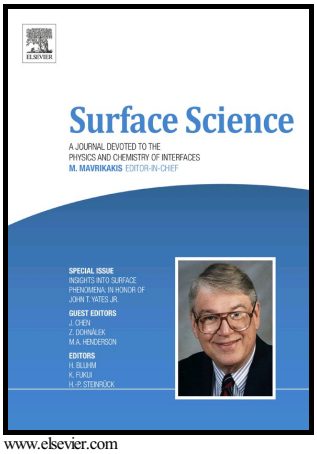

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ABSTRACT

Semiconducting metal oxide gas sensors have attracted growing interest as a result of their outstanding performance in the bio and industrial applications. Nevertheless, the sensing mechanism is yet not totally understood. In this study, we extensively investigate the adsorption mechanism of acetone molecule on ZnO-based thin film sensors by performing ab initio density functional theory calculations and employing quantum molecular dynamic simulations. Since the sensitivity of a metal oxide sensor is exceedingly depends on molecular oxygen exposure and operating temperature, we explore the competitive adsorption of acetone and oxygen molecule on the most stable orientation of ZnO surface $(10\bar{1}0)$ at different temperatures. Results indicate that at elevated temperatures acetone gains required thermal energy to remove preadsorbed