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Adsorption and Gas-Sensing Characteristics of a Stoichiometric A-Fe_2O_3 (0 0 1) Nano Thin Film for Carbon Dioxide and Carbon Monoxide with and without Pre-Adsorbed O_2

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The adsorption and gas-sensing characteristics of CO_2 and CO molecules on stoichiometric α-Fe_2O_3 (0 0 1) nano-thin film with and without pre-adsorbed O_2 molecules had beenstudied using the density functional theory (DFT) method. Without pre-adsorbed O_2 molecules, CO_2 molecule played as an acceptor and obtains electrons from stoichiometricα-Fe_2O_3 (0 0 1) nano-thin film. For the O_2 pre-adsorptionα-Fe_2O_3 (0 0 1) nano-thin film system, the CO_2 molecule alsoplayedas an acceptor. However, less number of electrons was transferred to CO_2 molecule ascompared to pre-adsorbed O_2 molecule. Different from CO_2 molecule, CO molecule always played as a donor forα-Fe_2O_3 (0 0 1) nano-thin film system with and without pre-adsorbed O_2. The theoretical results verify that the CO molecule can react with lattice or adsorbed oxygen of α-Fe_2O_3 (0 0 1) nano-thin film. The electrons transferred to the stoichiometric α-Fe_2O_3 (0 0 1) nano-thin film from CO molecule/new formed CO_2 molecule were more than that of transferred to the O_2 pre-adsorption α-Fe_2O_3 (0 0 1) nano-thin film. For stoichiometric or O_2 pre-adsorption α-Fe_2O_3 (0 0 1) nano-thin film, the CO_2 and CO moleculesexhibited opposite behaviors ofcharge transformation. In addition, pre-adsorbed O_2 molecules displayed competitive adsorption with CO_2 or CO molecule. The pre-adsorbed O_2 molecules hinder electron transfer to CO_2 molecule fromα-Fe_2O_3 (0 0 1) nano-thin film or hinder electron transfer toα-Fe_2O_3 (0 0 1) nano-thin film from CO molecule. Theoretical results demonstrate that the (0 0 1) surface of α-Fe_2O_3 materials could be prepared as adsorbents or gas sensors for CO_2 and CO molecules. Their structures were stable after CO_2 molecules were adsorbed or after the reaction of CO molecules withlattice or adsorbed oxygen ofα-Fe_2O_3 (0 0 1) nano-thin film.

Biography:

Changmin Shi was born in May 26, 1986. He received his B.S. degree in Condensed Matter Physics (2010-2015) from Shandong University. At present,he worked as a teacher in Institute of Condensed Matter Physics, School of Physics and Electric Engineering, Linyi University.