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Article

CO_2 Adsorption on H_2OÃƒÂ¢Ã‚Ã‚Â•Saturated BaO(1ÃƒÂ¢Ã‚Ã‚Â‰0ÃƒÂ¢Ã‚Ã‚Â‰0) and Induced Barium Surface Dissociation

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Abstract

CO_2 adsorption on a barium oxide (BaO) surface saturated with a monolayer of H_2O molecules was studied; a monolayer of H_2O molecules on the BaO surface exhibits nondissociative or dissociative adsorption. During the nondissociative reaction, a hydroxyl ionÃƒÂ¢Ã‚Ã€Ã‚•terminated surface is produced, resulting in the formation of barium hydroxide ($Ba(OH)_2$) on the surface. The $Ba(OH)_2$ from the substrate associates with the tightly bound CO_2 molecule, resulting in the formation of barium carbonate ($BaCO_3$). In contrast, during the dissociative H_2O adsorption, a hydrogenÃƒÂ¢Ã‚Ã€Ã‚•terminated surface is produced, which strongly adsorbs CO_2 molecules. The H_2O molecules on a fully saturated BaO surface (containing multiple layers of H_2O molecules) readily aggregate, and Ba dissociation takes place on the hydrated surface, possibly resulting in a surface containing Ba defects.

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