
Adsorption of carbon dioxide and methane on graphene with a high titanium coverage

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ABSTRACT

Using density functional theory and molecular dynamics to explore the adsorption of CO₂ and CH₄ at atmospheric pressure and 300 K we found that both adsorb on a graphene layer modified with titanium at high metal coverage (C₂Ti). The first dissociates to CO and O when adsorbed. The second is not dissociated and desorbs at 600 K.

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