First-principles calculation for adsorption of CH_4 on NiO (110) surface

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First principle calculation for adsorption of CH4 on NiO catalyst surface was performed. Various configurations were considered, and the adsorption energy was calculated for each case. Furthermore, calculations have been made on how adsorption configurations and energy change when CO_3^{2-} ions are present together. These calculations show that CO_3^{2-} ions can change the adsorption energy of CH4. This study will contribute to the conversion of C1 gas using electrochemical catalyst in the future.