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First-principles investigation of CO2 absorption on III-nitride surfaces YING-CHIN CHEN, HONG GUO, McGill Univ — Photon-induced chemical transformation of CO2 is a very interesting direction of green-house gas reduction. An accurate description of electronic structure at the interface between CO2 and the photocatalytics is important for understanding the process of artificial photosynthesis. In this work we report density functional theory (DFT) and many-body GW calculations to investigate CO2 adsorption on III-nitride semiconductor surface. The adsorption geometry is determined at the DFT level and the electronic structure is investigated at both DFT and GW levels. A detailed illustration of how the molecular orbital is renormalized is addressed.

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