Supporting Information for

Modelling molecular adsorption on charged or polarized surfaces: a critical flaw in common approaches

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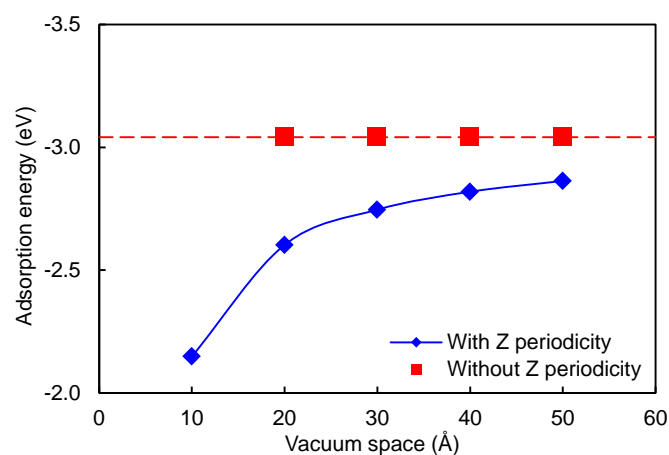
Belgium

CHARGED HEXAGONAL BN

Figure S1: Convergence dependence of CO_2 adsorption energies on charged *h*-BN on the vacuum space for both fully as partially periodic cells.
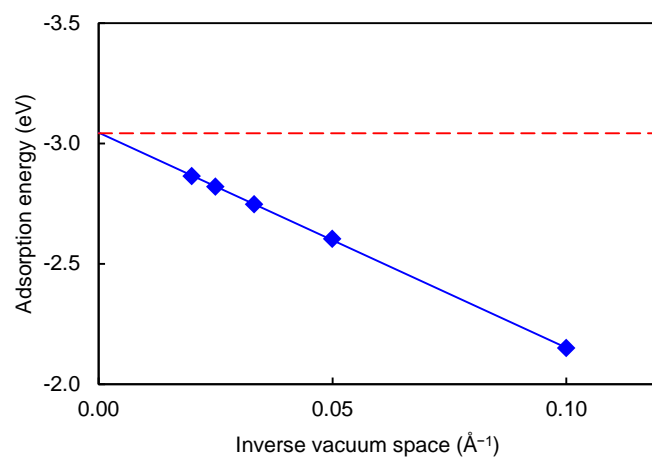
Figure S2: Extrapolation of CO_2 adsorption energies on charged *h*-BN for both fully as partially periodic cells to infinite vacuum.

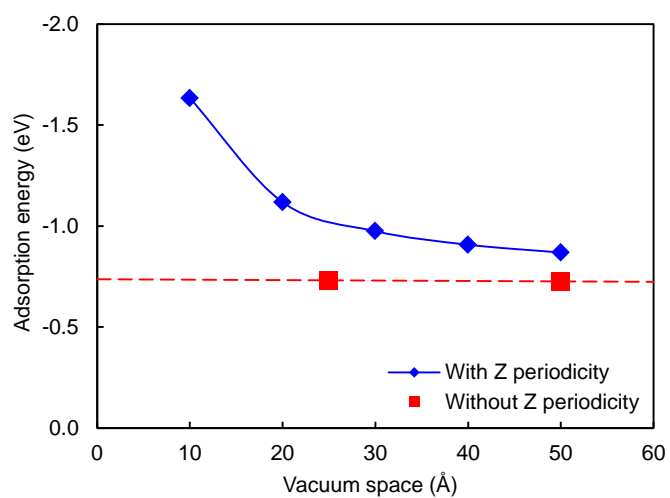## HEXAGONAL BN SUBJECTED TO AN ELECTRIC FIELD

Figure S3: Convergence dependence of electric field-enhanced CO_2 adsorption energies on *h*-BN on the vacuum space for both fully as partially periodic cells.
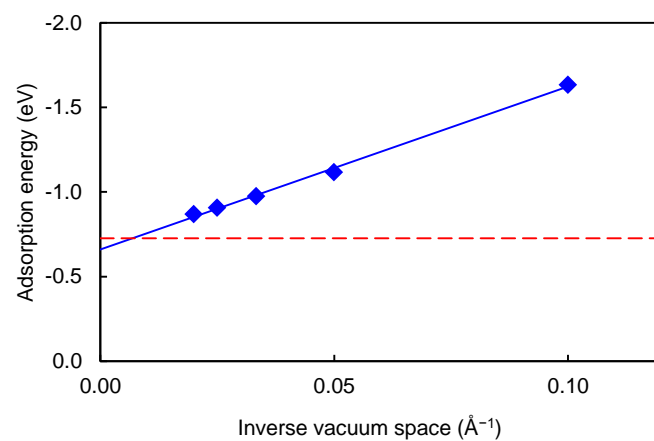
Figure S4: Extrapolation of electric field-enhanced CO_2 adsorption energies on *h*-BN for both fully as partially periodic cells to infinite vacuum.