Supporting Information for Adsorption Study of a Water Molecule on Vacancy-Defected Nonpolar CdS Surfaces

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1. Local DOS of S-atoms neighboring the V_{Cd} in bulk CdS

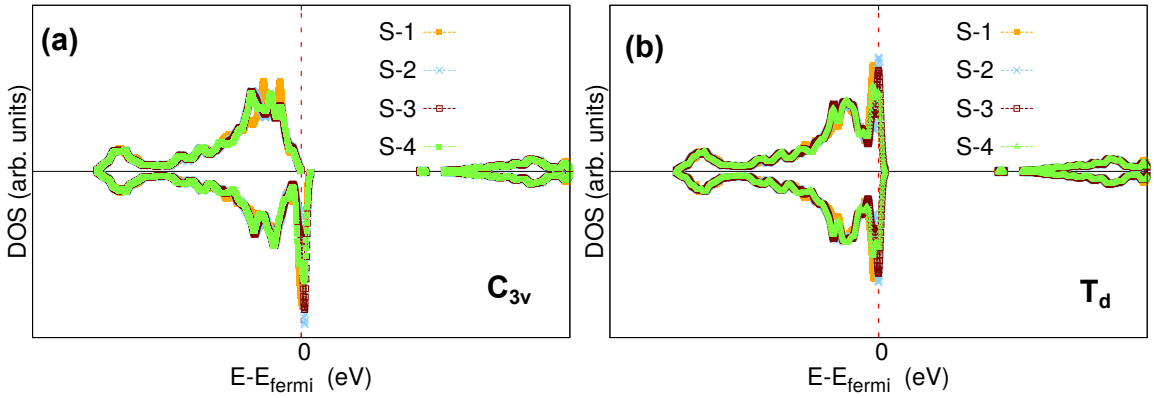

Figure S1: (a) and (b) are the spin-resolved LDOS of anions neighboring the V_{Cd} site in bulk CdS for the C_{3v} and T_d configurations, respectively. The atom S-1 in both the figures is the site along which the V_{Cd}-S bond is parallel to c-axis.

Figure S1 shows how the change in local geometry causes a change in the electronic states in the valence band, resulting into two types of magnetic states. From Fig.S1 (a), the difference in the electronic states of S-1 in comparison to other three S-sites validates the C_{3v} local point symmetry of the defect; whereas, for the T_d case in Fig.S1 (b), all the neighboring atoms have equivalent electronic structure.