Defect-engineering of 2D dichalcogenide VSe_2 to enhance ammonia sensing: Acumens from DFT Calculations

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Supporting information

Table S1. Adsorption energies for the adsorption of NH_3 on VSe_2 at different sites

System	Site for placing N atom of NH_3 on VSe_2 above 2 Å from surface	Adsorption energy (eV)
VSe_2+NH_3	V atom	0.124
VSe_2+NH_3	Se atom	0.135
VSe_2+NH_3	V-Se bond	0.218
VSe_2+NH_3	Centre of hexagonal ring consisting of V and Se atoms	0.147