Supplementary materials

The possible formation of magnetic FeS\textsubscript{2} phase in two-dimensional MoS\textsubscript{2} matrix

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Figure S 1 – The chosen atomic geometries of cluster FeS$_2$ in MoS$_2$ structure for different concentration. a) 2H-MoS$_2$ uniform structure, b) 2H cluster FeS$_2$ in 2H MoS$_2$ structure, c) 1H cluster FeS$_2$ in 2H MoS$_2$ structure, d) 1H cluster FeS$_2$ in 1H MoS$_2$ structure. The molybdenum, iron and sulfur atoms are presented in red, blue and green, respectively.
Figure S 2 – The atomic geometries of the most stable $\text{Fe}_{x}\text{Mo}_{1-x}\text{S}_2$ structures, predicted by evolutionary algorithm USPEX. The molybdenum, iron and sulfur atoms are presented in red, blue and green, respectively.