Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary materials

The possible formation of magnetic FeS_2 phase in two-dimensional MoS_2 matrix

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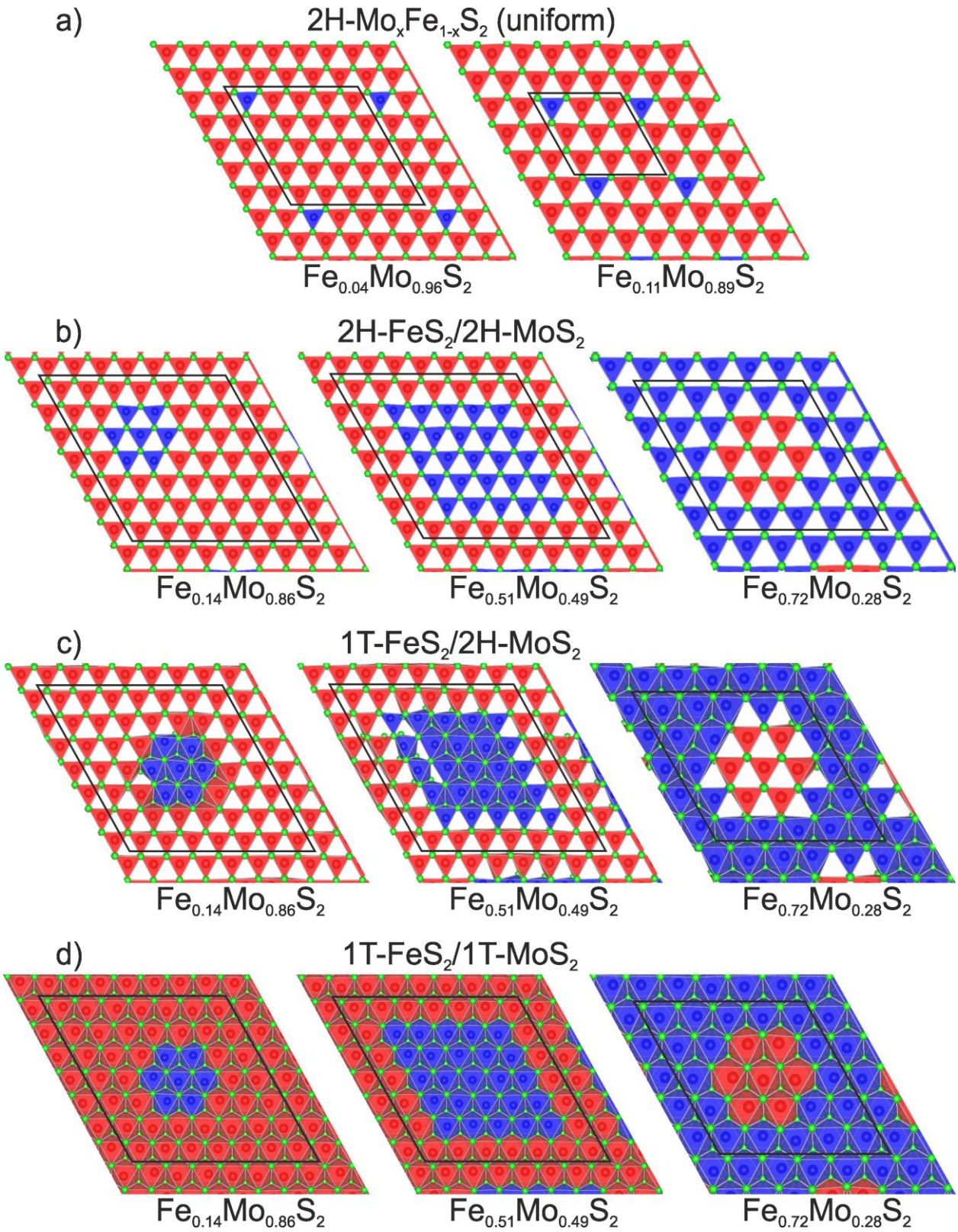

Figure S 1 – The chosen atomic geometries of cluster FeS_2 in MoS_2 structure for different concentration. a) 2H-MoS_2 uniform structure, b) 2H cluster FeS_2 in 2H MoS_2 structure, c) 1H cluster FeS_2 in 2H MoS_2 structure, d) 1H cluster FeS_2 in 1H MoS_2 structure. The molybdenum, iron and sulfur atoms are presented in red, blue and green, respectively.

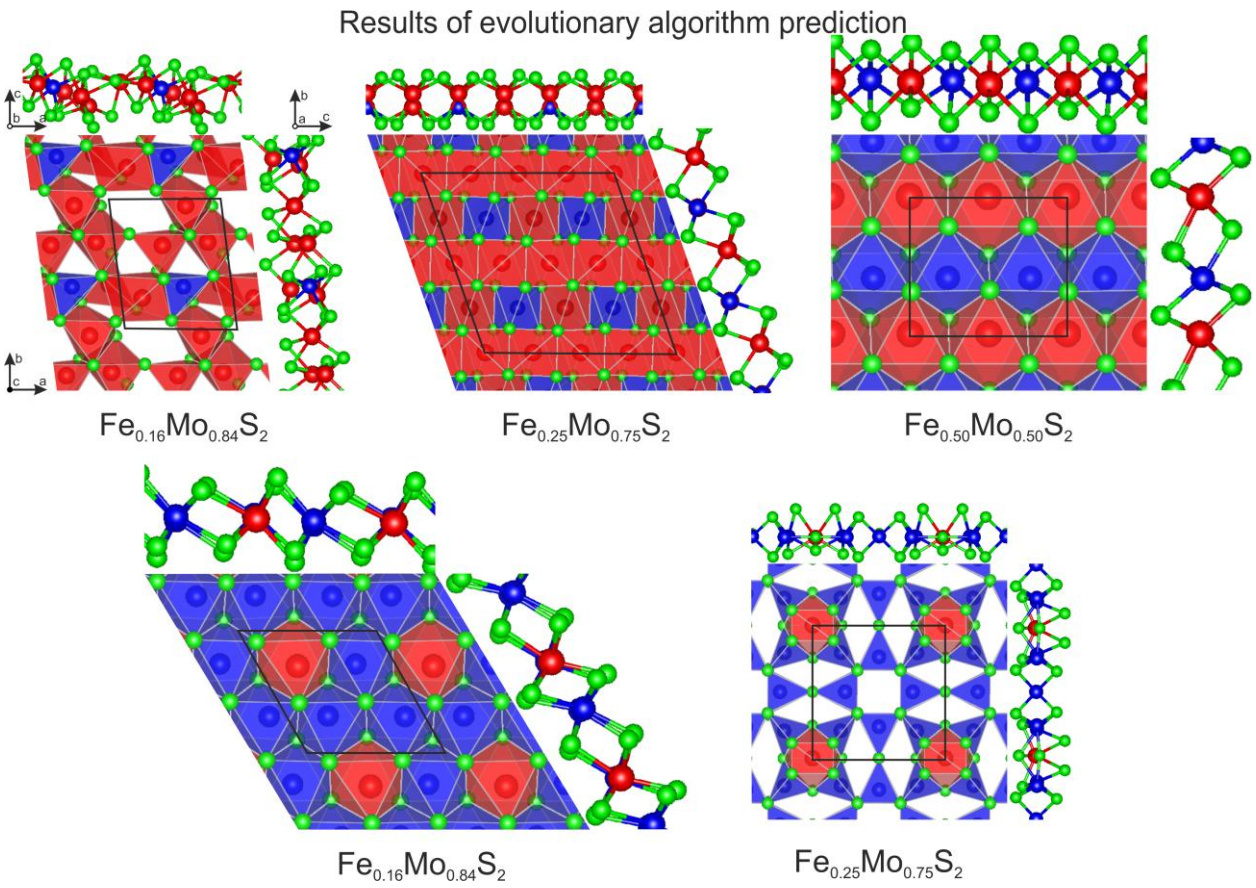

Figure S 2 – The atomic geometries of the most stable $Fe_xMo_{1-x}S_2$ structures, predicted by evolutionary algorithm USPEX. The molybdenum, iron and sulfur atoms are presented in red, blue and green, respectively.