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Band gap closure in MnS under pressure

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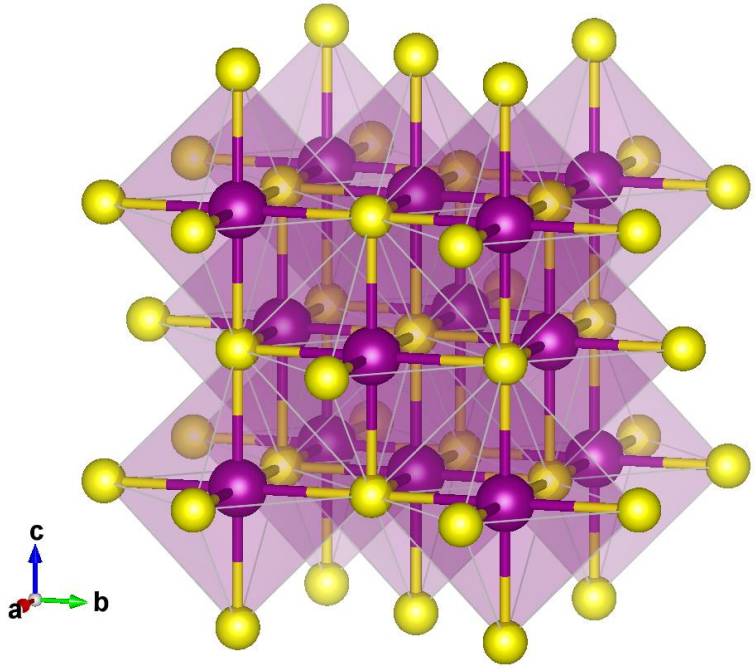
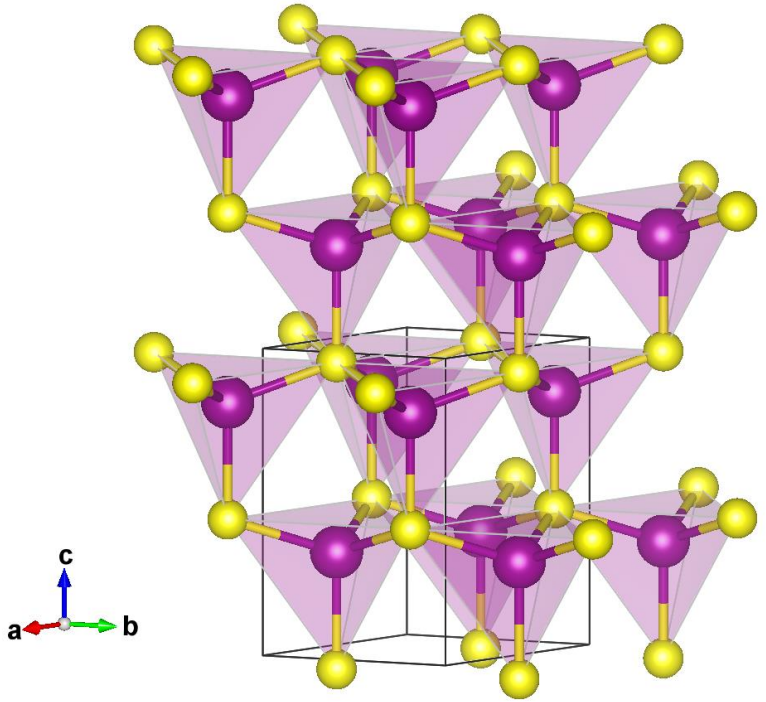
Crystal structure of MnS

α-MnS	γ-MnS
	
$Fm\bar{3}m$ a = b = c = 5,254 Å [1] α = β = γ = 90°	$P6_3mc$ a = b = 3,96 Å, c = 6,4 Å [2] α = β =90°, γ = 120°

[1] Wakabayashi J. , et al., Journal of the Physical Society of Japan, 25, 227-233 (1968)
[2] Schwartz A., et al., Materials Research Bulletin, 2, 375-380 (1967)

Methods

- Density Functional Theory (DFT)
  - Generalized Gradient Approximation (GGA)
    - Pseudopotentials of PBEsol (Perdew-Burke-Ernzerhof) [3]
- Density functional-based method that takes into account correction for Coulomb interaction parameter U (DFT+U) [4]
- Software package: Quantum Espresso [5]

[3] Perdew J.P. et al., Phys. Rev. Lett. 9, 767 (1996)
[4] Anisimov V.I., Gunnarsson O., Physical Review B 43, 7570-7574 (1991)
[5] Giannozzi P. et al., J. Phys.: Condens. Matter. 29, 465901 (2017)

The electronic structure of α-MnS with electronic correlations

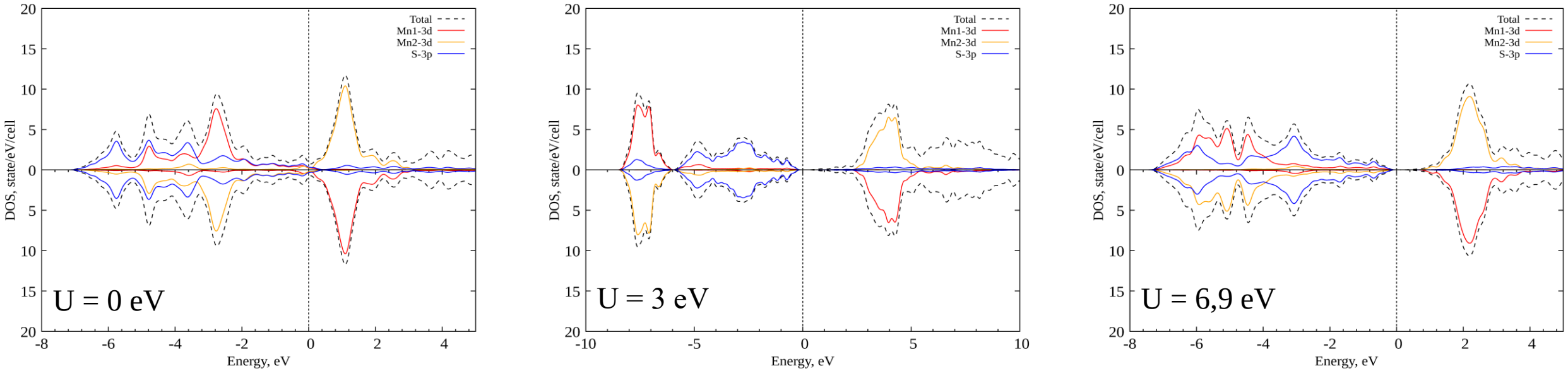


Fig. 1. The density of states of α-MnS for different values of the U parameter. The plot is shifted relative to the Fermi energy, shown by a vertical dotted line at zero energy.

The electronic structure of α-MnS for different volumes

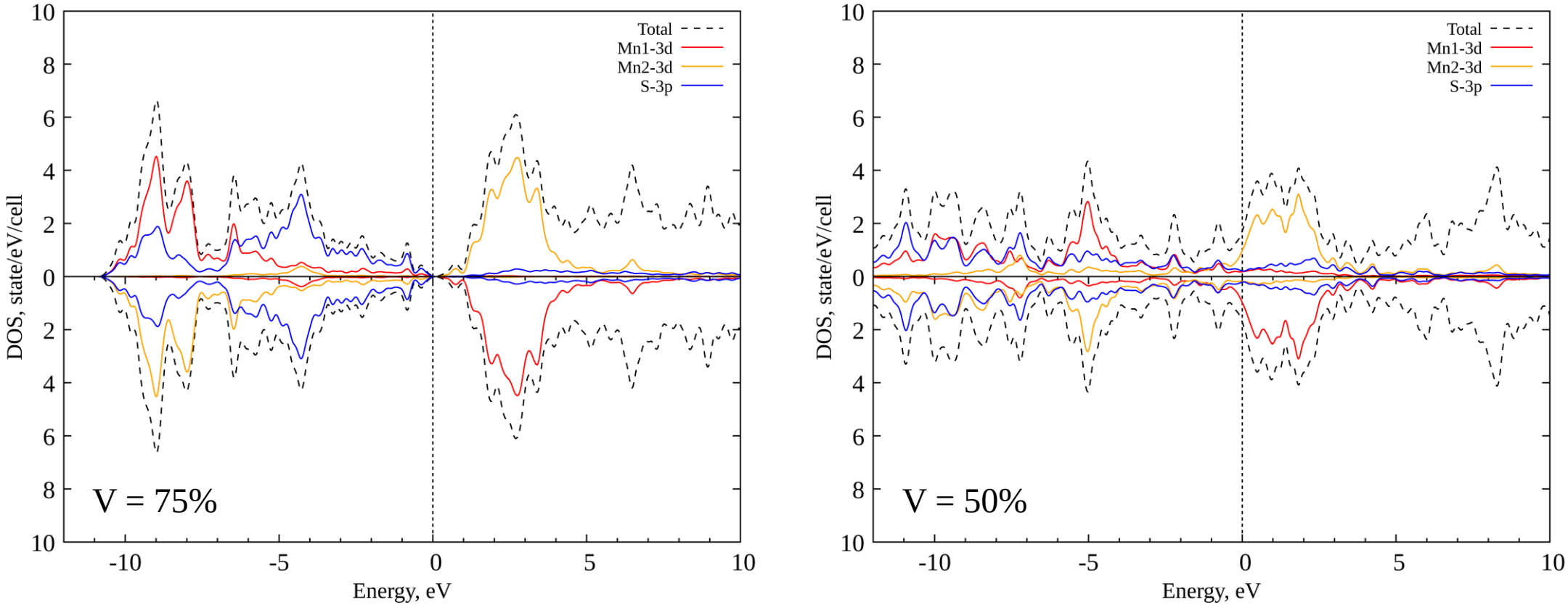


Fig. 2. The density of states of α-MnS for different volumes and U = 6,9 eV. The plot is shifted relative to the Fermi energy, shown by a vertical dotted line at zero energy.

The electronic structure of γ-MnS with electronic correlations

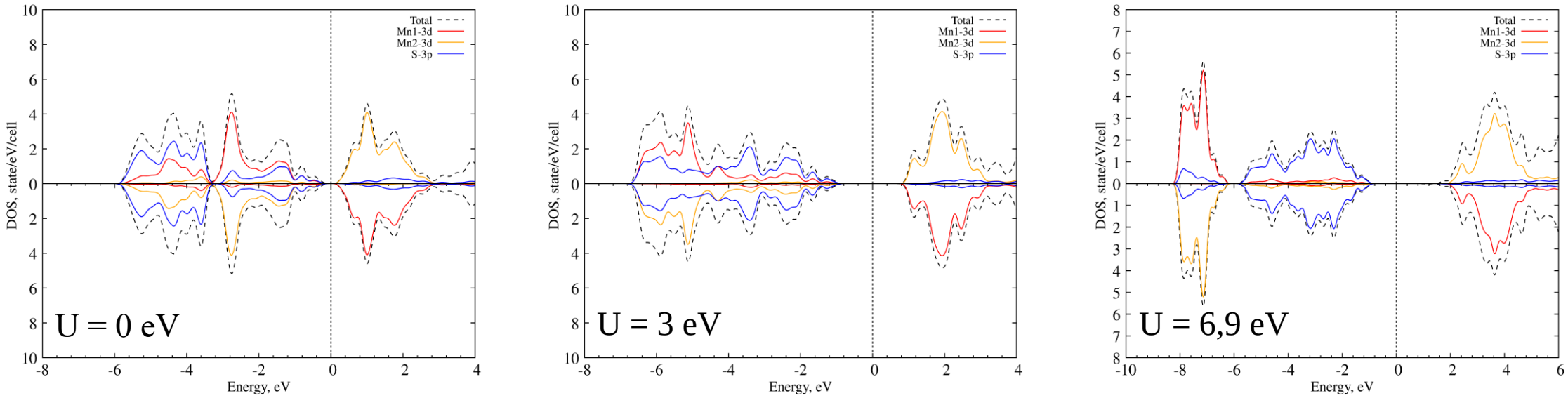


Fig. 3. The density of states of γ-MnS for different values of U. The plot is shifted relative to the Fermi energy, shown by a vertical dotted line at zero energy.

The electronic structure of γ -MnS for different volumes

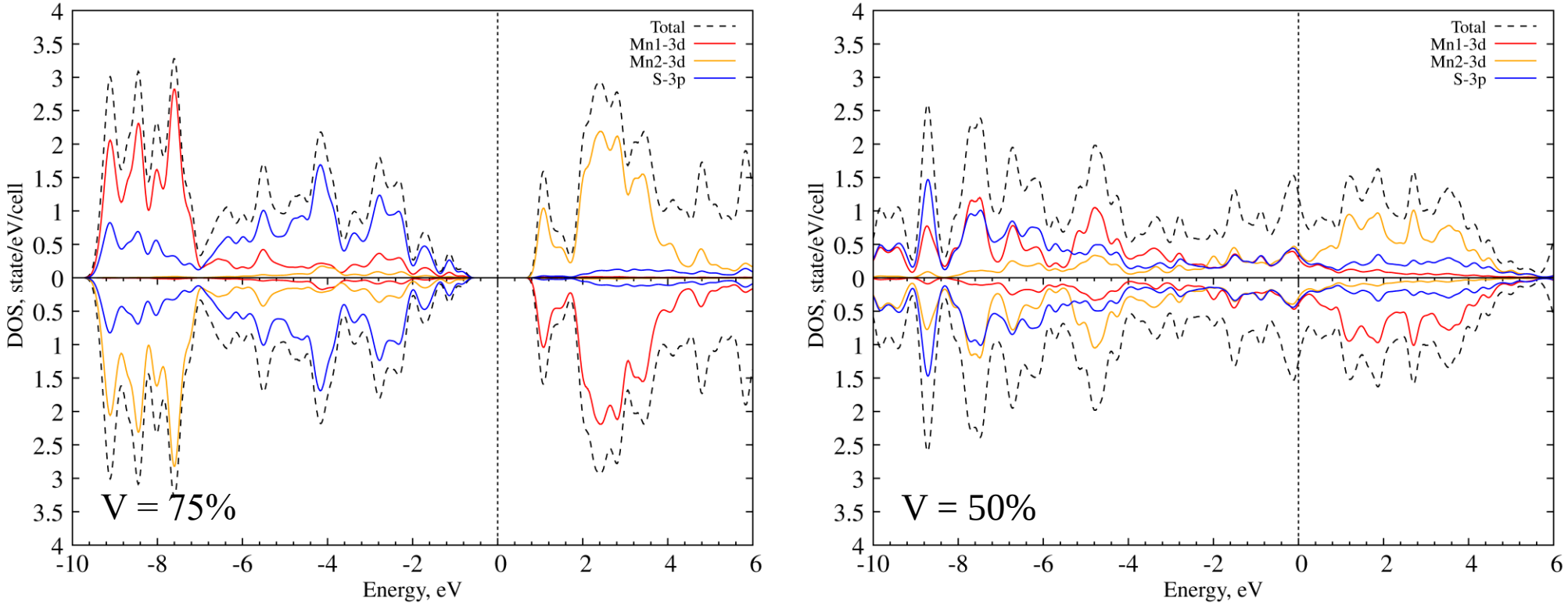


Fig. 4. The density of states of γ-MnS for different volumes and U = 6,9 eV. The plot is shifted relative to the Fermi energy, shown by a vertical dotted line at zero energy.

Conclusions

- Our theoretical studies have revealed a metal-insulator phase transition for α-MnS, with an increase in the Coulomb interaction parameter.
- As well as the insulator-metal phase transition for α-MnS and γ -MnS when the volume of the unit cell is compressed to 50% of the volume under normal conditions.

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Thank you for your attention!