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Large-scale atomistic simulations of MgO exsolution process driven by machine learning potentials

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The origin of the Earth's ancient magnetic field is a long-standing problem. MgO may exsolve out of the liquid outer core to drive core convection and power the early geodynamo. Due to experimental and computational challenges, the exact amount of MgO exsolved out of the Earth's core remains controversial. Here we utilize an iterative learning scheme that combines enhanced sampling, feature selection, and deep learning to develop a unified machine learning potential of *ab initio* quality for the MgO-Fe system valid over a wide pressure-temperature range (Deng et al., 2023). The potential enables direct, large-scale simulations of MgO exsolution process from metallic melts at the Earth's core-mantle boundary conditions. The resulting trajectories are further analyzed using the Gibbs dividing surface method to determine element partition coefficients. Implications for the energetics of the early geodynamo and core-mantle interactions will be discussed.

References

Deng, J., Niu, H., Hu, J., Chen, M., Stixrude, L., 2023. Melting of $MgSiO_3$ determined by machine learning potentials. Phys Rev B 107(6), 064103. doi.org/10.1103/PhysRevB.107.064103.