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(De)formation of mantle minerals: Insights from atomic-scale simulations

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Minerals are the building blocks of the Earth. Knowledge of their formation and evolution is needed to understand both the structure and the dynamics of our planet. As only the upper part of the crust is accessible to direct sampling, models of the deep interior of the Earth rely on a combination of geophysical observations, laboratory experiments and simulations. Here, we use various atomic scale simulation methods to shed light on the structure and thermodynamic stability of mantle minerals, defects in their crystal structure and on the mechanisms of diffusion and shear deformation. These simulation techniques are unique in the sense that they provide simultaneous access to atomic structures and to thermodynamic or transport properties. On the other hand, chemical and structural complexity of relevant Earth materials require both substantial computational resources and efficient though still accurate simulation methods. We therefore use a combination of classical and first-principles molecular modeling methods, accelerated dynamics techniques such as metadynamics and sometimes educated guess. A big challenge for future research will be to establish the link between the atomic and the continuum scale, especially for modeling one- or two-dimensional crystal defects and for modeling plastic deformation.

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