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Modeling of thermo-chemical properties of the sub-solidus MgO-FeO binary, under Earth's lower mantle conditions

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The stability field of the Mg-wüstite solid solution, (Mg,Fe)O, under high PT conditions, has been investigated by performing quantum mechanical calculations combined with statistical thermodynamics.
The interest in this field comes from the consideration that the Mg-wüstite is the second most abundant phase in the Earth's lower mantle. A thoughtful understanding of the thermodynamic stability of this phase under deep mantle conditions is thus crucial for developing accurate models of the Earth's interior and the importance of drawing a complete picture of the stability fields of the Mg-wustite solid solution, especially at high pressure/temperature regimes, is straightforward.
The experimental research in this field can be conveniently integrated by computational methods that allow not only to explore the extreme conditions that cannot be realized in a laboratory but also to express the mixing energies of the system as a function of the different factors affecting it.
In the light of the above considerations, the present work has been undertaken where the thermo-chemical properties of the (Mg,Fe)O solid solution, over a wide PT range, have been modelled. Calculations have been performed by means of quantum mechanical and semi-empirical techniques by applying different external hydrostatic pressures in the range 0-140 GPa. The effect of the different spin configurations have been taken into account by exploring both the diamagnetic (low spin, S=0, NM) and antiferromagnetic (high spin, S=2, AFM) cases.
The obtained energies have been then employed for the parameterization of the excess energy by the interaction parameters determined via Cluster Expansion (CE) method.
The critical values of Pressure and Temperature beyond which the AFM-model, which is energetically more convenient in the low pressure regime, ends up promoting decomposition into MgO-FeO end members, have been determined for each investigated composition over the MgO-FeO binary.
The proposed approach allowed us to achieve a comprehensive picture of the principles underlying the stability of (Mg,Fe)O-solid solution, as a function of those aspects that primarily affect its reactivity, i.e. pressure, temperature, composition and iron spin-configuration, and to determine, therefore, those conditions which favors the stability of the solid solution.