Simulations identify how critical elements distribute in abundant mineral ores

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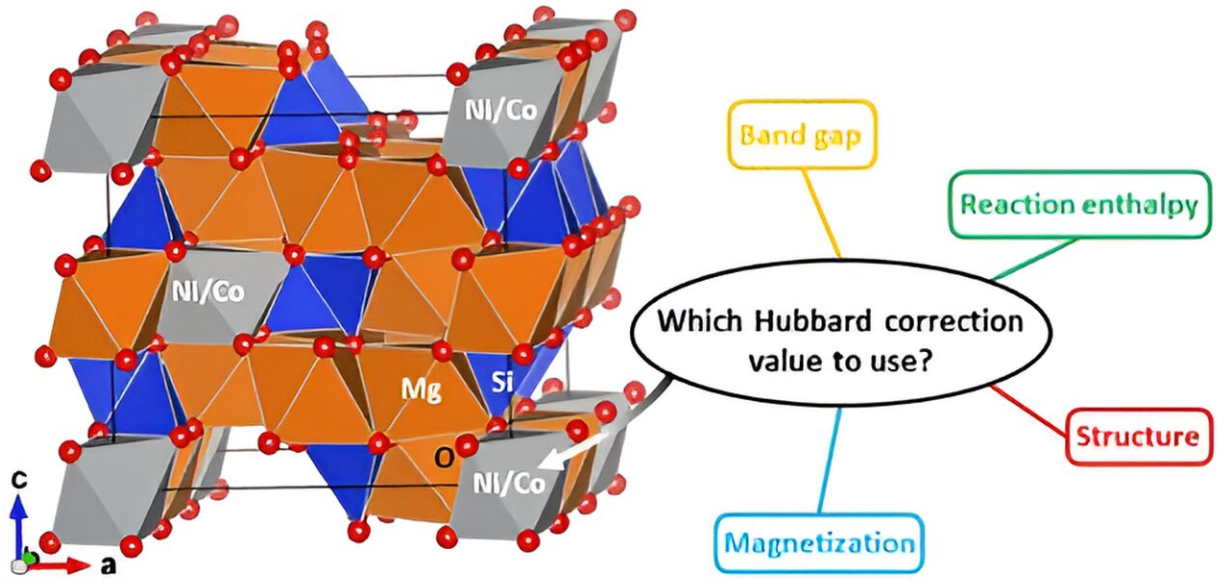

Credit: *ACS Earth and Space Chemistry* (2024). DOI: 10.1021/acsearthspacechem.3c00370

Nickel (Ni) and cobalt (Co) are critical elements for modern technologies, with high-grade Ni and Co ores becoming increasingly scarce. Mafic and ultramafic deposits are low-grade, abundant alternatives to traditional Ni and Co ores. However, new methods that make Ni and Co extraction and recovery from these deposits economically viable are needed.

Researchers used ab initio molecular dynamics simulations to identify how Ni and Co incorporate in forsterite (Mg_2SiO_4), common in mafic and ultramafic rocks. The results show that, of the two cation sites of forsterite (M1 and M2), Ni and Co incorporation in the M1 site is preferred. This preference is diminished in natural samples with low Ni/Co concentrations relative to literature data on more highly concentrated samples.

The findings are published in the journal *ACS Earth and Space Chemistry*.

Carbonation of silicate minerals like forsterite could improve the economic viability of Ni and Co extraction and recovery from low-grade ores by lowering ore-processing costs and helping the mining industry reach net-zero CO_2 emissions.

This work identifies how forsterite incorporates Ni and Co with atom-level detail, beneficial information for scientists developing new extraction and recovery methods. These results will help researchers understand how silicate minerals like forsterite react with CO_2 during carbonation and guide efforts to improve Ni and Co extraction and recovery.

More information: Michel Sassi et al, Ni and Co Incorporation in Forsterite: A Density Functional Theory Study with Hubbard Correction, *ACS Earth and Space Chemistry* (2024). DOI: 10.1021/acsearthspacechem.3c00370

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