

## Accumulation of Cr and Ni in clays and nanocrystalline iron oxides from ultramafically-derived sediments in northern California, USA

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We are investigating the role that weathering and transport play in the bioaccessibility of geologically sourced and potentially toxic Cr and Ni in northern California. These elements are enriched (1700 to 10,000 mg kg<sup>-1</sup> Cr and 1300 to 3900 mg kg<sup>-1</sup> Ni) in ultramafic (UM) rocks (primarily serpentinite) in the Coast Range and Sierra Nevada foothills, and transported to the adjacent Sacramento Valley. As a result, valley soil contains 80 to 1420 mg kg<sup>-1</sup> Cr and 65 to 224 mg kg<sup>-1</sup> Ni compared to U.S. geometric means for soil of 37 and 13 mg kg<sup>-1</sup>, respectively. Nickel in UM source rocks and soils is hosted by serpentine minerals (lizardite, antigorite, and chrysotile) and is more labile compared to Cr, which primarily resides in the highly refractory mineral chromite ([Mg, Fe<sup>2+</sup>][Cr<sup>3+</sup>, Al, Fe<sup>3+</sup>]<sub>2</sub>O<sub>4</sub>).

Based on scanning electron microscopy/energy dispersive x-ray (SEM/EDX) and transmission electron microscopy (TEM) studies, we find evidence for dissolution and mineralogical alteration of Cr and Ni host phases during *in situ* weathering of serpentinite, erosional transport, and continuing alteration in Sacramento Valley soil. Results from SEM on soils overlying UM source rocks reveal decreased Cr content in dissolution etch textures along edges of chromite grains. Analysis by TEM of the <2 μm fraction of UM and valley soils document Cr and Ni in clay minerals (smectite/illite) and nanocrystalline iron oxides. The clay minerals in the <2 μm fraction of UM soils contain Cr and Ni up to 0.72 and 0.86 wt% respectively and the nanocrystalline iron oxides contain 1.16 wt% Cr and 2.81 wt% Ni. Valley soils (<2 μm) contain Cr and Ni values as high as 700 and 3300 mg kg<sup>-1</sup> in clays and 1500 and 1800 mg kg<sup>-1</sup> in iron oxides, respectively.

Particle size analysis of the soils (<2mm) determined the clay-sized fraction to be 30% and 25% of the soil for source and valley soils, respectively. Although the majority of Ni and Cr in soils is still in serpentine and refractory chromite minerals, the presence of etching and dissolution of primary minerals and metal-rich clays and nanocrystalline Fe oxides is evidence that a significant fraction has been transformed to more bioaccessible forms.

## Nuclear quantum effects in water

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The importance of nuclear quantum effects in hydrogen bonded systems has been underlined by recent experimental measurements of the proton momentum distribution [1-2]. In this work, we utilize open path integral Car-Parrinello molecular dynamics simulations in order to compute the proton momentum distribution and assess the impact of nuclear quantum effects in several phases of water [3-5]. We find that our results are in good agreement with the experimental momentum distributions measured in liquid water and hexagonal ice. It is also found that the inclusion of nuclear quantum effects systematically improves the agreement of first-principles simulations of liquid water with experiment. In addition, we study phases of high-pressure ice that exhibit symmetric hydrogen bonds and quantum tunneling. The symmetric hydrogen bonded phase possesses a narrowed momentum distribution as compared with a covalently bonded phase, in agreement with recent experimental findings. The signatures of tunneling that we observe are a narrowed distribution in the low-to-intermediate momentum region, with a tail that extends to match the result of the covalently bonded state. The transition to tunneling behavior shows similarity to features observed in recent experiments performed on confined water.

- [1] G.F. Reiter, J.C. Li, J. Mayers, T. Abdul-Redah, & P. Platzman (2004) *Braz. J. Phys.* **34**, 142. [2] C. Andreani, D. Colognesi, J. Mayers, G.F. Reiter, & R. Senesi (2005) *Adv. Phys.* **54**, 377. [3] J.A. Morrone, V. Srinivasan, D. Sebastiani, & R. Car (2007) *J. Chem. Phys.* **126**, 234504. [4] J.A. Morrone & R. Car (2008) *Phys. Rev. Lett.* **101**, 017801. [5] J.A. Morrone, L. Lin, & R. Car (2009) *J. Chem. Phys.* **130**, 204511.