Importance of correlation effects in first-principles simulations of iron at high-pressure

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The importance of magnetic and correlation effects in high-pressure research is often overlooked. The usual motivation here is that under compression the overlap between localized states increases and so does the bandwidth W, while the local Coulomb repulsion U between those states is screened more efficiently. The reduction of U/W ratio is used to rationalize the neglect of electronic correlations beyond state-of-the art local density approximation (LDA) or semi-local generalized gradient approximation (GGA) at high-pressure conditions. Concerning magnetism, the Stoner theory becomes more realistic at very high temperature $T >> T_c$ (T_c is the Curie temperature) where the disappearance of local magnetic moments can be expected.

In particular, based on these arguments iron at the inner Earth's core conditions is modeled as non-magnetic within LDA-based approaches. To challenge this point of view, we have performed calculations with a new implementation of the dynamical mean-field theory (DMFT). It is based on a highly precise full-potential linear augmented plane wave (FLAPW) method for the band structure calculation combined with DMFT in conjunction with a continuous-time quantum Monte Carlo (CTQMC) impurity solver for treating the strong correlations [1]. The application of the methodology has shown anumbigously that inclusion of correlation effects beyond LDA/GGA has led to qualitatively new physical effects predicted in Fe at moderate, as well as at ultra-high pressure and temperature.

[1] Aichhorn *et al.* (2009) *Phys. Rev. B* **80**, 085101.

Cadmium isotopes in the western North Atlantic — GEOTRACES cruise PE319

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We present cadmium concentration and isotopic composition data for four depth profiles from GEOTRACES cruise PE319, which sailed from Scrabster, UK to Bermuda during April and May 2010, following the eruption of the Eyjafjallajoekull volcano in Iceland.

Recent Cd isotope data have shown that the cadmium biogeochemical cycle in the high nutrient, low chlorophyll (HNLC) regions of the Southern Ocean is controlled by both ocean circulation and primary production [1]. In contrast, the surface waters of North Atlantic subtropical gyre are considered oligotrophic for much of the year, and the high latitude (>55°N) North West Atlantic is seasonally HNLC [2].

Seawater samples, collected using a titanium frame and ultra clean sampling techniques [3], were analysed for cadmium isotopic composition and concentration using a double-spike technique using Thermal Ionization Mass Spectrometry (DS-TIMS) at MPI. One litre seawater samples were processed as described by Abouchami *et al.*[1]. Data are reported relative to our NIST SRM 3108 standard ($^{110}Cd/^{112}Cd$=0.520121±4 (2SD, n=14)).

Preliminary results from the Irminger Basin (at 64.0°N, 34.25°W) show relatively constant cadmium concentrations, with a mean concentration of 0.25 ± 0.02 nmol kg^{-1} in the upper water column. The $\varepsilon^{112/110}Cd$ show little variation, with a mean value of +2.9 ± 0.26, and are similar to those reported in surface waters from the Arctic and North Atlantic [4]. Additionally, the ratio of phosphate to cadmium concentration appears to be coherent with models and observations of this ratio at low phosphate concentrations [5]. These results are consistent with seasonal observations of hydrographic mixing and stratification in the region [6].

[1] Abouchami *et al.* (2011) *EPSL* **305**, 83–91. [2] Nielsdóttir *et al.* (2009) *GBC* **23**, GB3001. [3] De Baar *et al.* (2008) *Mar.Chem.* **111**, 4–21. [4] Ripperger *et al.* (2007) *EPSL* **261**, 670–684. [5] Boyle (1988) *Paleoceanography*, **3**, 471–489. [6] Holliday *et al.* (2006) *J. Marine Systems* **59**, 201–208.