First-principles calculations of the lattice thermal conductivity of the lower mantle

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The rate of loss of heat from Earth's core is controlled by the thermal conductivity of the minerals that comprise the overlying mantle. The heat-flux at the core-mantle boundary has implications for the thermal evolution of both the core and mantle, the size and stability of plumes, and magnetic field generation. As insulators, conduction in lower mantle phases is expected to be dominated by phonon transport. Estimates of the thermal conductivity of MgSiO3 perovskite, the most abundant phase, at core-mantle boundary conditions, vary significantly, with the phonon contribution reported to lie between 1.6 and 17 Wm⁻¹K⁻¹. In view of this, we have performed ab initio non-equilibrium molecular dynamics simulations to determine the lattice thermal conductivity of MgSiO₃ perovskite at lower mantle conditions, calculating it to be 6.5 ± 0.8 Wm⁻¹ K⁻¹, a value consistent with geophysical constraints on the thermal state at the base of the mantle. Our results suggest that the conductivity depends strongly on pressure, helping to explain the dynamical stability of superplumes, and weakly on temperature and composition, so that lateral variations in thermal conductivity at the base of the mantle are small.

Origin of methane to n-butane in marine sediments of the New Jersey shallow shelf

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Concentrations and stable carbon isotope compositions of C_1 to C_4 in pore fluids were measured in three cores (M0027A, M0028A and M0029A) of IODP Expedition 313 that targeted Mioscene sedimentary sequences up to 67 km off the coast of New Jersey, USA (Mountain et al. 2010), to understand processes related to gas geochemistry and carbon cycling in the investigated shallow shelf. Stable carbon isotope data and $C_1/(C_2+C_3)$ ratios suggest a biogenic origin of methane. If methane is produced by a biogenic process this could in principle also be the case for C_{2+} gases as suggested by Hinrichs et al. (2006). An alternative explanation could be low-temperature kerogen cracking (Rowe & Muehlenbachs 1999). Showing first data we discuss gas formation mechanisms including the potential source of the organic material, secondary alteration processes and the role of mixing of gases of different origin (biogenic versus thermal) at the investigated site.

[1] Hinrichs, K.U., Hayes, J.M., Bach, W., Spivackl, A.J., Hmelo, L.R., Holm, N.G., Johnson, C.G. and Sylva, S.P. (2006): Biological formation of ethane and propane in the deep marine subsurface. - Proceedings of the National Academy of Sciences of the United States of America 103:14684-14689. [2] Mountain, G., Proust, J.-N., McInroy, D., Cotterill, C., and the Expedition 313 Scientists (2010): Proceedings of the Integrated Ocean Drilling Program, Volume 313: Tokyo (Integrated Ocean Drilling Program Management International, Inc.).[3] Rowe, D., Muehlenbachs, A. (1999): Low-temperature thermal generation of hydrocarbon gases in shallow shales. – Nature (London) 398:61-63.