Molecular dynamics simulation of materials

MICHELE PARRINELLO[1*]

[1]ETH Zurich and Università della Svizzera Italiana, Lugano, Switzerland, parrinello@phys.chem.ethz.ch (*presenting author)

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The experimental study of systems under condition of high temperature and pressure provide a considerable challenge. Accurate and reliable computer simulations could be of great help in this area of science. However to reach this goal considerable technical difficulties need to be overcome. We present a number of methods developed in our laboratory that greatly help towards reaching this goal. We apply these techniquese to study the phase diagram of materials, structural phase transition and the nucleation of crystals from solution.

Fluctuations in Precambrian atmospheric and oceanic oxygen levels: a new Precambrian paradigm emerging?

C.A. PARTIN[1*], A. BEKKER[1], N.J. PLANAVSKY[2], B.C. GILL[3], C. LI[4], V. PODKOVYROV[5], A. MASLOV[6], K.O. KONHAUSER[7], G.D. LOVE[2], T.W. LYONS[2]

[1]University of Manitoba, Geological Sciences, Winnipeg, Canada, umpartin@cc.umanitoba.ca (* presenting author), bekker@cc.umanitoba.ca

[2]University of California, Riverside, Earth Sciences, U.S.A., planavsky@gmail.com, glove@ucr.edu, timothyl@ucr.edu

[3]Virginia Tech, Geosciences, Blacksburg, U.S.A., bcgill@vt.edu

[4]China University of Geosciences, Key Laboratory of Biogeology and Environmental Geology, Wuhan, China, chaoli@cug.edu.cn

[5]Russian Academy of Sciences, Institute of Precambrian Geology and Geochronology, St. Petersburg, Russia, vpodk@mail.ru

[6]Russian Academy of Sciences, Zavaritskii Institute of Geology and Geochemistry, Ekaterinburg, Russia, Maslov@igg.uran.ru

[7]University of Alberta, Earth and Atmospheric Sciences, Edmonton, Canada, kurtk@ualberta.ca

The Precambrian atmosphere and oceans are traditionally thought to have undergone a progressive, gradual increase in oxygen content after ~2.4 Ga [1]. This gradual transition from anoxic to oxidizing conditions is assumed to have occurred in two incremental steps, one at the beginning, and one at the end of the Proterozoic Eon. Emerging data require a change to this paradigm. Enrichments of the redox-sensitive element uranium in organic matter-rich shales through time shows that the Earth's surface oxidation had a more dynamic and unexpected history. Archean shales show very low [U] (<10 ppm, average of 3.8 ppm), consistent with a large U sink in anoxic oceans. The Great Oxidation Event (GOE) is accompanied by a rapid increase in maximum [U], up to 60 ppm, which likely reflects the onset of strong oxidative continental weathering releasing soluble U and expansion of oxygenated environments in the oceans. The initial rise of atmospheric oxygen ~2.4-2.32 billion years ago was followed by a dramatic decline to less oxidizing conditions during the Middle Proterozoic, beginning after the cessation of the Lomagundi carbon isotope excursion at ~2.05 Ga, when [U] in shales returned to near-to-crustal levels (average of 3.2 ppm). The subsequently established, steady-state low-oxygen mode persisted for nearly one billion years, terminating with a second oxygenation event in the latest Neoproterozoic, when [U] in shales demonstrate a dramatic increase, up to 94 ppm, by 551 Ma. Utilizing the ubiquitous geological shale record, U concentrations reveal Earth's dynamic path to its presently well-oxygenated atmosphere-ocean system, with unprecedented temporal resolution. We will present evidence for a precipitous rise and (previously unrecognized) fall in atmospheric oxygen early in the Proterozoic, which is in direct contrast to conventional models predicting a unidirectional oxygen rise. With this new paradigm in mind, future models will need to reexamine the links between the co-evolution of life and the chemical composition of the Precambrian oceans.

[1] Kump, L. (2008) *Nature* **45**, 277-278.