Reverse chemistry of iron in the deep Earth

Xiaoli Wang,[1,2,3] Xiaolei Feng,[4,5] Jianfu Li,[1] Dalar Khodagholian,[6] Matthew G. Jackson,[2*] Frank J. Spera,[2] Simon A. T. Redfern[5,4*] and Maosheng Miao[6,3*]

[1]*Institute of Condensed Matter Physics, Linyi University, Linyi 276005, People's Republic of China*

[2]*Department of Earth Science, University of California Santa Barbara, Santa Barbara, California 93110, United States*

[3]*Beijing Computational Science Research Center, Beijing 100084, People's Republic of China*

[4]*Center for High Pressure Science and Technology Advanced Research (HPSTAR), Shanghai 201203, China*

[5]*Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge, CB2 3EQ, UK*

[6]*Department of Chemistry and Biochemistry, California State University, Northridge, California 91330, United States*

The distribution and abundance of both major and trace elements in the Earth's interior provide a record of its formation and evolution[1,2]. An understanding of this record demands knowledge of the chemical affinity of the elements and their compounds under the high-pressure conditions of Earth's interior. For many years, our understanding of such affinities has been predominantly biased by low-pressure observations that are of dubious applicability to Earth's deep mantle and core[3]. Here we conduct a systematic computational study of the propensity of *p*-block elements to chemically bind with iron under high pressures ranging from ambient conditions to that of Earth's core. We show that under increasing pressure, iron tends to reverse its chemical nature, changing from an electron donor (reductant) to an electron acceptor, and oxidizes *p*-block elements in many compounds. Such reverse chemistry has a significant impact on the stoichiometries, bond types and strengths, structures and properties of iron compounds under deep planetary conditions. High pressure greatly enhances bonding to iron for many *p*-block elements that are conventionally labeled lithophile or chalcophile[1,4], making them highly siderophile.