



Direct *ab initio* iron melting at high pressure

Anatoly B. Belonoshko(1,2), Anders Rosengren(2), Leonid Burakovsky(3), Dean L. Preston(4) and Börje Johansson(1,5)

(1) Institute of Materials Science and Engineering, Stockholm, Sweden, (2) Department of Physics, AlbaNova University Center, The Royal Institute of Technology, Stockholm, Sweden, (3) Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, U.S.A., (4) Physics Division, Los Alamos National Laboratory, Los Alamos, New Mexico, U.S.A., (5) Condensed Matter Theory Group, Department of Physics, Uppsala University, Uppsala, Sweden (anatoly@fysik.uu.se / Fax: +46 018 4713524)

Iron is the main constituent of the Earth's core. Considerable efforts have been made to clarify the properties of iron at high pressure and temperature. These efforts have not only clarified the iron phase diagram, but also produced a number of discrepancies, the most noticeable of them being the difference between the so called "low" and "high" melting curves. We will report the results of *ab initio* molecular dynamics direct simulations of iron melting at high pressure applying projector-augmented wave implementations of density functional theory. The results provide support to the high melting curve.