July 8, 17:00-18:00
Online

Seminar

Understanding Atoms in Tight Places

Martin Rahm

Chemistry and Chemical Engineering, Chalmers University of Technology, Sweden

Speaker introduction

Martin received his Master degree in Chemistry and Chemical Engineering from the Royal Institute of Technology in 2006. He remained to complete a PhD in Physical Chemistry in 2011, with the Quantum Chemistry group of Tore Brinck and the polymer chemistry group of Eva Malmström. During 2011 – 2013, Martin worked as a postdoctoral researcher at the University of Southern California, and pursued modeling and synthesis work in the group of Karl Christe. From 2014 – 2016, he worked as a postdoc in the combined theoretical chemistry and condensed matter physics group of Roald Hoffmann and Neil Ashcroft at Cornell University. He is currently an Associate Professor at Chalmers University of Technology. Martin's research interests include chemical bonding, high pressure chemistry, energetic materials, astrobiology and quantum computation.

Invited by Dr. Christian Tantardini, Research Scientist at CEST.

Seminar abstract

Following a brief introduction to our research activities at Chalmers, this presentation focuses on new ways to rationalize chemistry under conditions of extreme pressure. A quantum mechanical model that can describe the effect of uniform compression of single atoms by a nonreactive chemical medium is presented. Results for 93 atoms up to 300 GPa include several characteristics: (1) the electronic configuration of the ground state isolated atoms, which arguably defines the very nature of the periodic table; (2) the central chemical notion of electronegativity, so useful for rationalizing chemical bonding and, in particular, polarity and charge transfer; and (3) the Van der Waals radii of atoms, central to our understanding of structure and bonding. Comparison with experimental equations of state and structure will be discussed along with predictions of inversed polarity and reactivity under compression. An open interactive web application, the Atoms Under Pressure Database, will also be demonstrated.