# MM 12: Invited talk Todorova

Time: Monday 15:00–15:30 Location: BAR 205

**Invited Talk** MM 12.1 Mon 15:00 BAR 205

**From weakened chemical bonds to materials breakdown: An ab initio perspective** — •Mira Todorova — Max-Planck-Insitut für Eisenforschung, Düsseldorf, Germany

Materials failure mechanisms originate at the microscopic scale. Density functional theory (DFT) calculations have proven to be a versatile tool, providing access to the most fundamental level of forming, weakening or breaking of chemical bonds. A major challenge in the practical realization is the structural and chemical complexity of real-world materials. As will be discussed, fully ab initio computed chemical potentials open a powerful way of transferring the inherently microscopic DFT results to the engineering/device scale. It will be shown that these potentials can be utilised to successfully address various phenomena related to materials failure. The presentation will exemplify this by outlining the steps and the insight which can be achieved by applying these approach on two key failure mechanisms - liquid metal embrittlement [1] and corrosion of galvanized steels [2].

[1] K.-D. Bauer, M.Todorova, K. Hingerl, and J. Neugebauer, Acta Mater. **90**, 69 (2015).

[2] M.Todorova and J. Neugebauer, Farad. Discussions **180**, 97 (2015).