« AgNW and AgNP Network" Serenade Labex Seminar
Monday February 13, 2017
ISTerre, Grenoble

Participants (confirmed): Ben Gilbert (LBNL), Kevin Rosso (PNNL), Sylvia Lehmann (ISTerre), Isabelle Michaud-Soret (LCBM/CEA) , Giulia Veronesi (LCBM/CEA), Marianne Marchioni (LCBM/CEA), Aurélien Deniaud (LCBM/CEA), Djadidi Toybou (LITEN/CEA/ISTerre), Caroline Celle (LITEN/CEA), Géraldine Sarret (ISTerre), Ana Elena Pradas (ISTerre-ESRF), German Montes-Hernandez (ISTerre), Delphine Tisserand (ISTerre), Chrysovalanto Irene (ISTerre-US, l'après midi), Elise Eymard-vernain (LCBM/CEA, l'après midi), Laurent Charlet (ISTerre)

To be confirmed: Michel Campillo (ISTerre), Alejandro Fernandez-Martinez (ISTerre)

Place: ISTerre, Campus UGA, Dolomieu conference room, 3d floor (https://isterre.fr/isterre/contact-et-acces/article/isterre-grenoble?lang=en)

Note that the Seminar by Kevin Rosso will be give in the Conference room (with video in streaming, organized by CEREGE), ISTerre 1st floor

Programme (20 min talks, 10 min questions):

9:00 Coffee
9:30 General Introduction: Laurent Charlet (ISTerre) and Ben Gilbert (LBNL)

10:00 Djadidi Toybou (CEA-ISTerre): Mechanism governing AgNW synthesis and shape
10:30 Géraldine Sarret (ISTerre): AgNP grafting on textile fibers, a feasibility study
11:00 Géraldine Sarret (ISTerre) and Elise Eymard-Vernain (CEA): Interaction of AgNP with bacilus subtillis
11:30 Marianne Marchioni: Sorption of organo thiol molecules on AgNP; dissolution/aggregation effect

12:30 to 1:30 Lunch break

1:30 Ana-Elena Pradas: Synthetic and natural sulfudation of AgNP
2:00 Sylvia Lehmann: Dermal toxicity of AgNW
2:30 Ben Gilbert and Laurent Charlet: Achievements and Challenges of the Network

3:00: Coffee break

3:30 - 4:30 p.m. Kevin Rosso "**Advances in Understanding the Kinetics of Electron Transfer Across Mineral/Water Interfaces**" in ISTerre Conference Room (1st floor)

Advances in Understanding the Kinetics of Electron Transfer Across Mineral/Water Interfaces

Kevin M. Rosso

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Bio: Dr. Kevin Rosso is a Laboratory Fellow and the Associate Director for the Physical Sciences Division, Geochemistry Group. Dr. Rosso joined Pacific Northwest National Laboratory in 1998 and is recognized for his work to creatively address long-standing problems in mineral surface chemistry related to reactivity and electron exchange at the mineral-water interface. Dr. Rosso's current projects include the following: (1) characterizing the kinetics and mechanisms of elementary charge and ion transport processes in redox transformation of iron oxide minerals, (2) predicting molecular-scale electron transfer kinetics in microbially-mediated reduction of bioavailable iron in subsurface environments, (3) studying mechanisms of heterogeneous reduction of contaminant U(VI) and Tc(VII) by Fe(II)-bearing minerals, (4) simulation of coupled charge and ion transport in transition metal oxide electrodes for advanced materials applications, (5) probing mechanisms and kinetics of mineral transformation to metal carbonates for geological carbon sequestration, and (6) studying mechanisms of uptake and retention of uranium in sediments.

Keywords: electron transfer, iron oxide, ferrihydrite, goethite, hematite, magnetite, small polaron, Marcus theory

Abstract: Electron transfer (ET) is one of the most fundamental and essential processes in nature as well as technological frontiers, playing a commanding role in enzymatic function, photocatalysis, corrosion, mineral precipitation and dissolution. Research in new energy systems development, functional materials design, and in understanding the biogeochemical cycling of elements requires robust experimental and computational approaches to unravel rate controlling factors at mineral/water interfaces at the atomic scale. This presentation will overview current and emerging methods applied to a variety of ET-mediated interfacial processes, emphasizing the multi-disciplinary complex problem of aqueous Fe(II)/Fe(III)-oxide interaction. At redox gradients in natural waters, as well as in corrosion fronts in metals or at poised iron oxide interfaces, changes in the electrochemical potential impact iron valence distribution, and, in turn, phase stabilities and aqueous solubilities. In almost all cases, aqueous Fe(II) is juxtaposed against sparingly soluble Fe(III) solids. Highly soluble Fe(II) catalyzes recrystallization of hydrous ferric oxides into more crystalline and stable Fe(III)-oxyhydroxides and oxides. Beyond very informative high resolution electron and atomic force microscopies, and synchrotron X-ray absorption and scattering analyses, isotopically labelled Fe tracer studies show that recrystallization is facile and involves a moving front through solid interiors. Polaronic electron mobility through these solids appears to play a key role, linking spatially remote interfacial ET donor and acceptor site across nanophase crystallites. More than a decade of multiscale multiphysics simulation studies of the thermally activated hopping of self-trapped charge carriers in iron oxides and oxyhydroxides shows the predominance of local coordination for setting the magnitude of the reorganization energy, and of bridging (hydr)oxo ligands for setting the strength of electronic coupling. The critical roles of bulk and interfacial structural defects on the rates of ET and phase transformation overall thus follow naturally and intuitively. The central set of Fe(II)/Fe(III) interfacial ET examples that will be discussed illustrate significant new insights into factors controlling ET dynamics generally, and help define a path for resolving a wide range of multidisciplinary interfacial ET problems in the future.