

Modélisation de systèmes électrochimiques par dynamique moléculaire

Mathieu Salanne

Laboratoire PHENIX, Sorbonne Universités, UPMC
Maison de la Simulation, CNRS/CEA/INRIA/Univ. Paris Saclay





Sels fondus pour le cycle électronucléaire



Stockage électrochimique de l'énergie



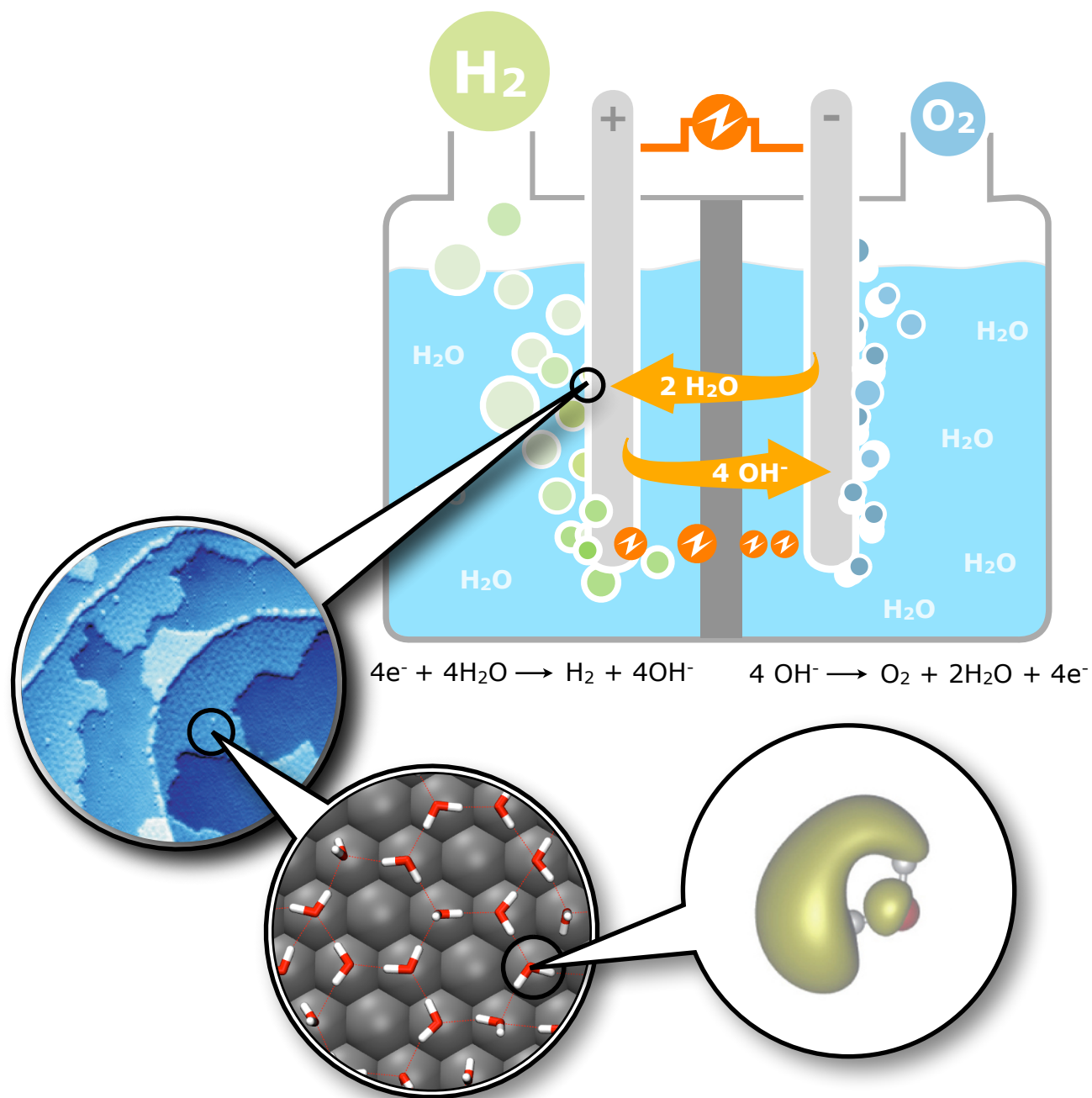
Recyclage de matériaux pour l'énergie

Synthèse / Électrochimie / Caractérisation / **Modélisation**

Stockage électrochimique de l'électricité



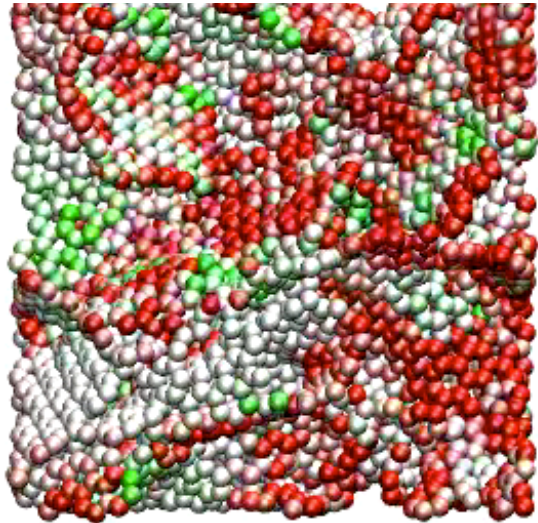
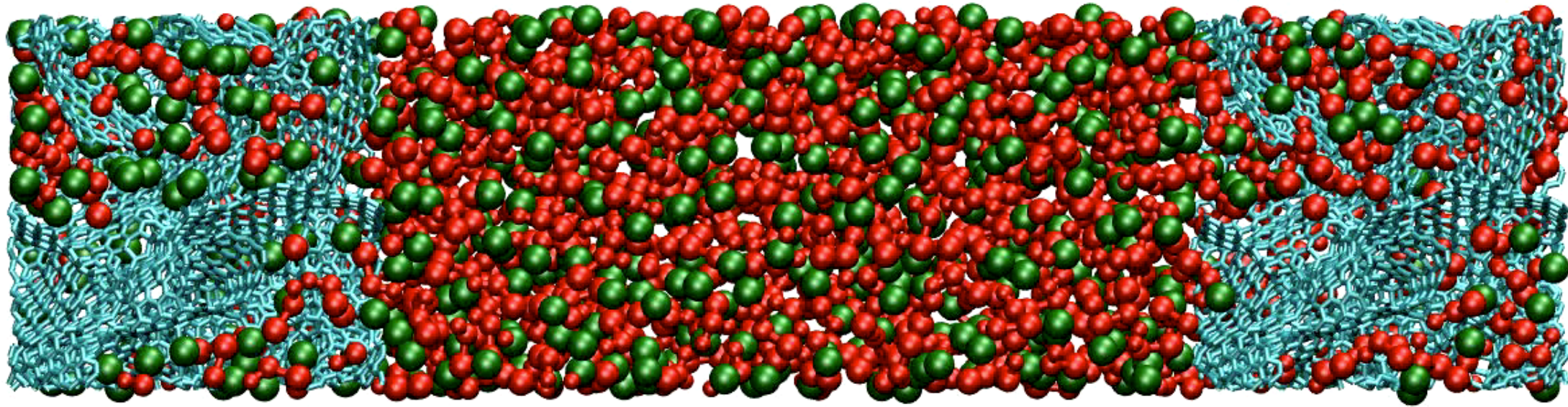
Modélisation de systèmes électrochimiques



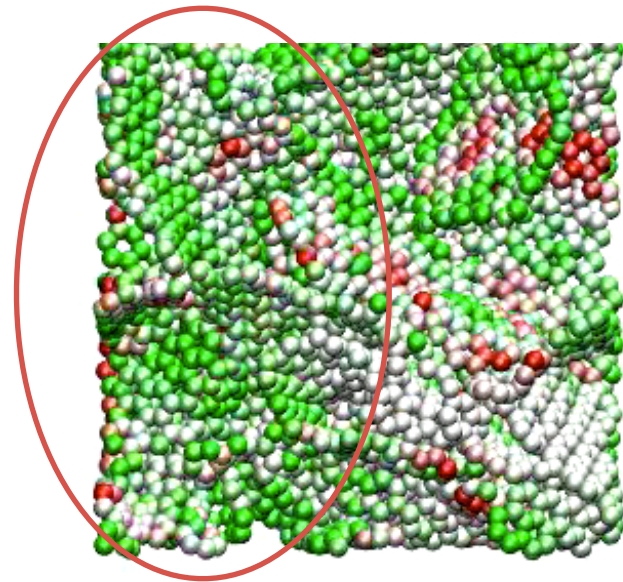
Liquides ioniques



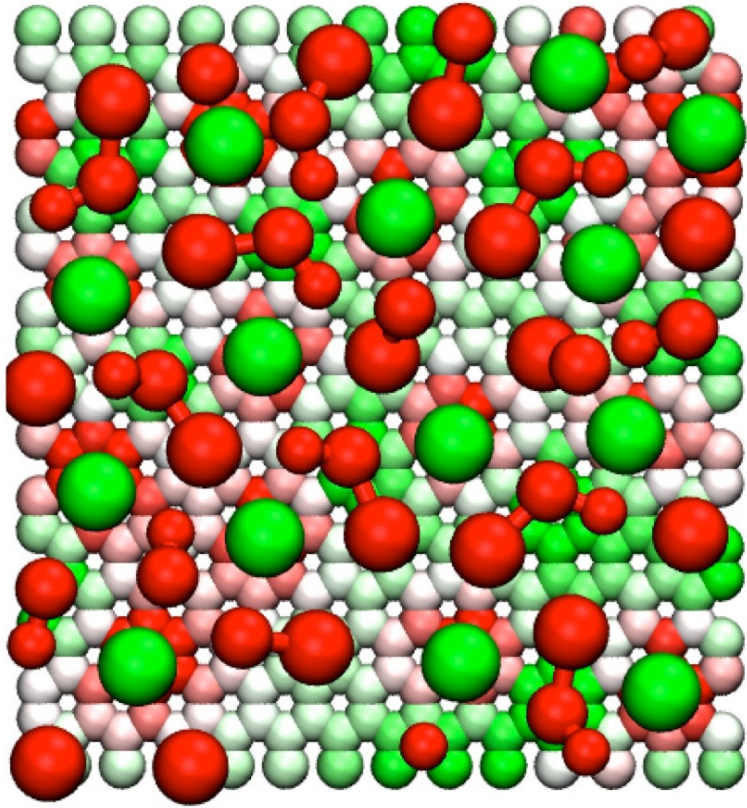
Supercondensateurs carbone/carbone



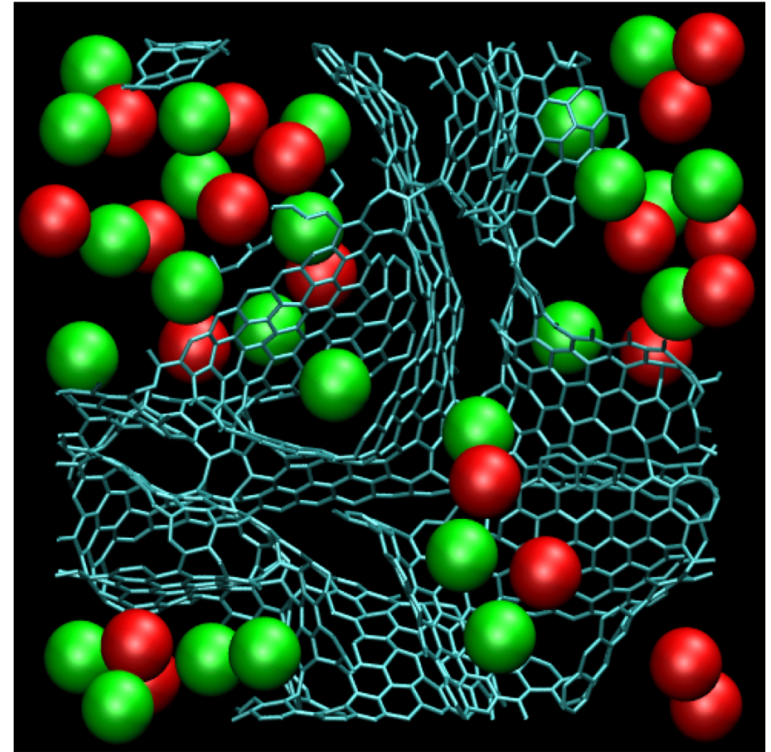
Accumulation
d'électrons



Carbones nanoporeux (thèse C. Merlet)

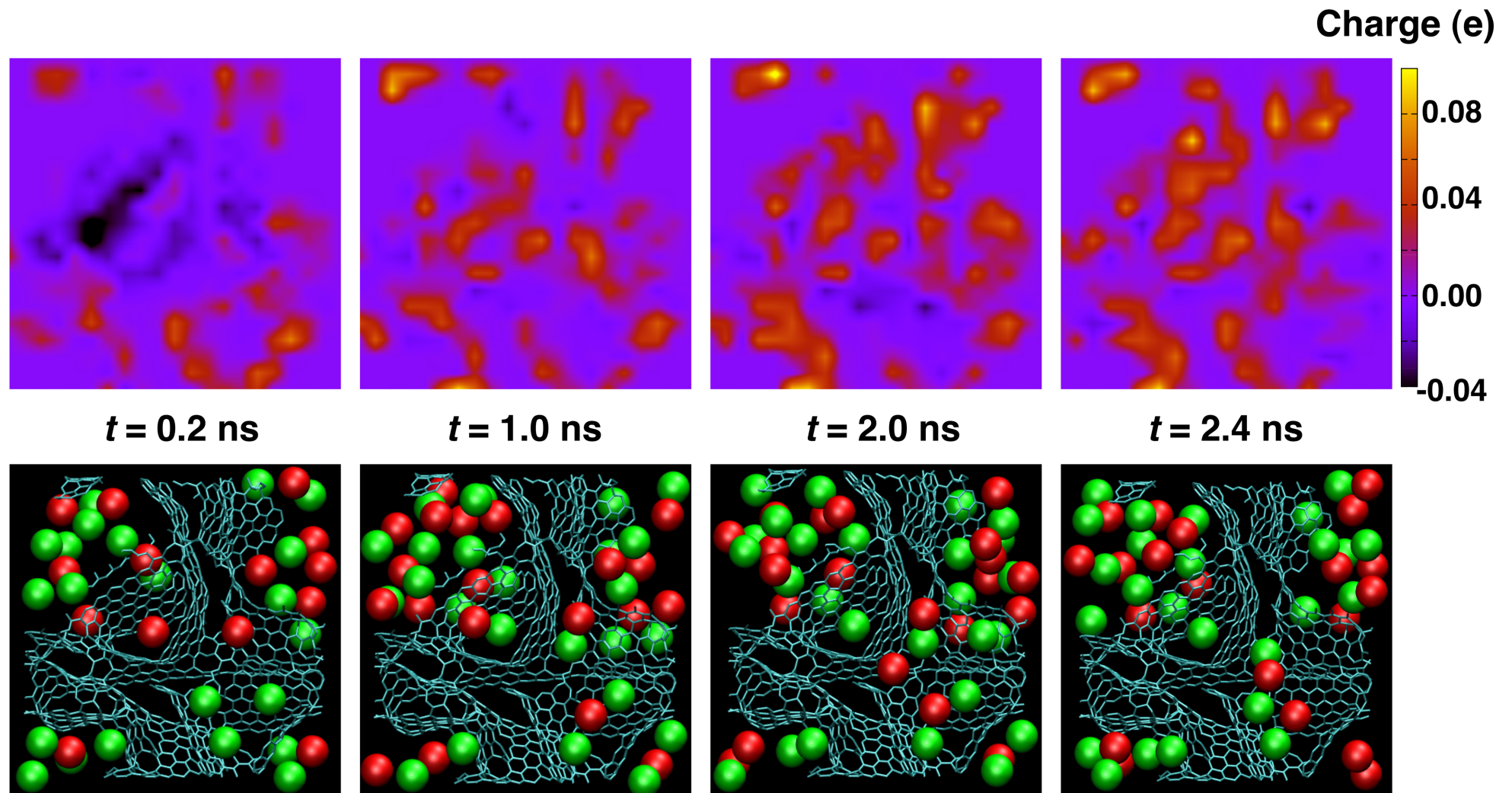


Graphite: 60 F g⁻¹

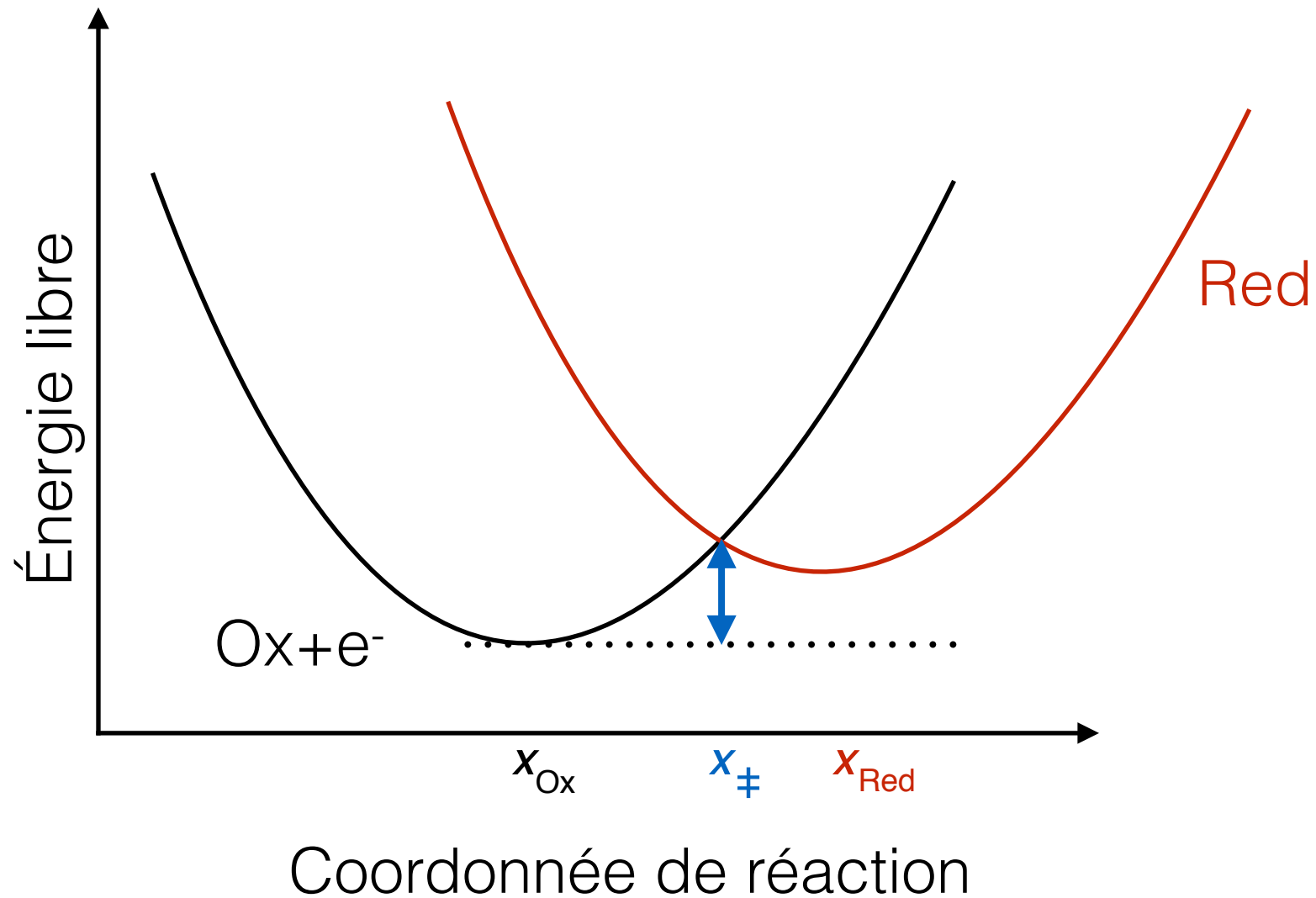


Nanoporeux: 180 F g⁻¹

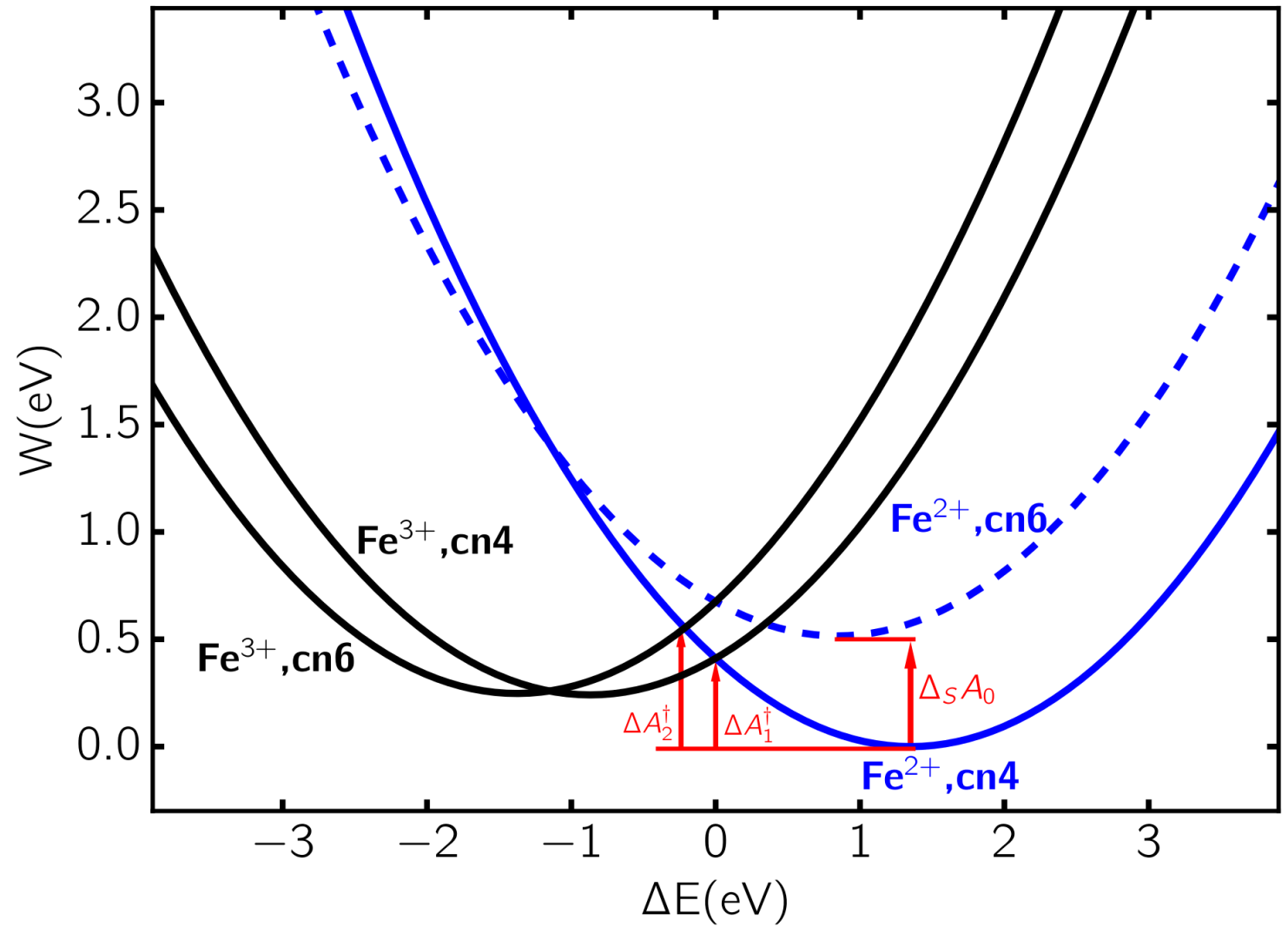
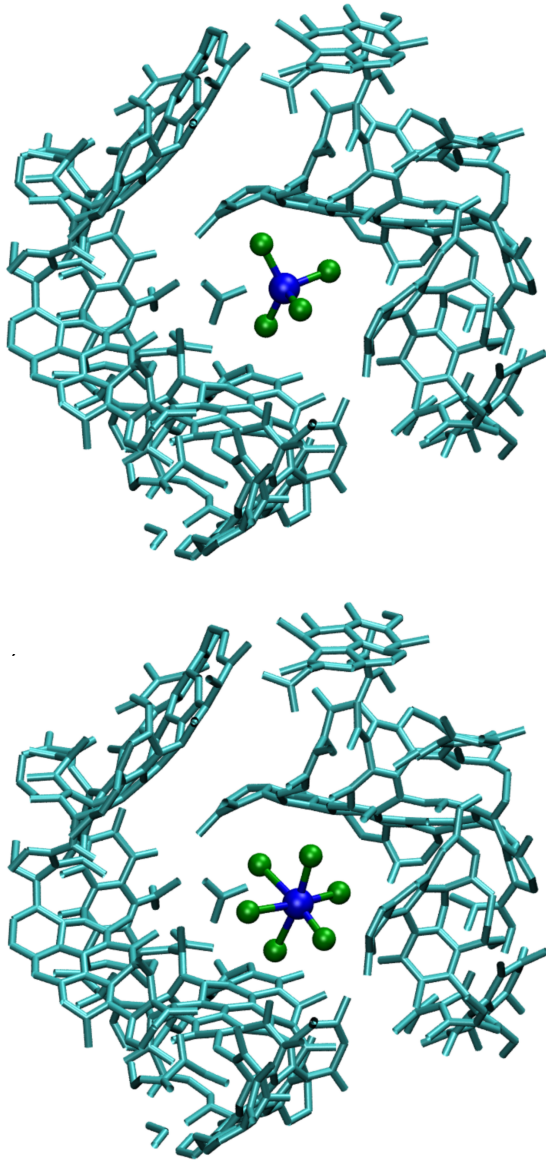
Dynamique de charge (thèse C. Péan)



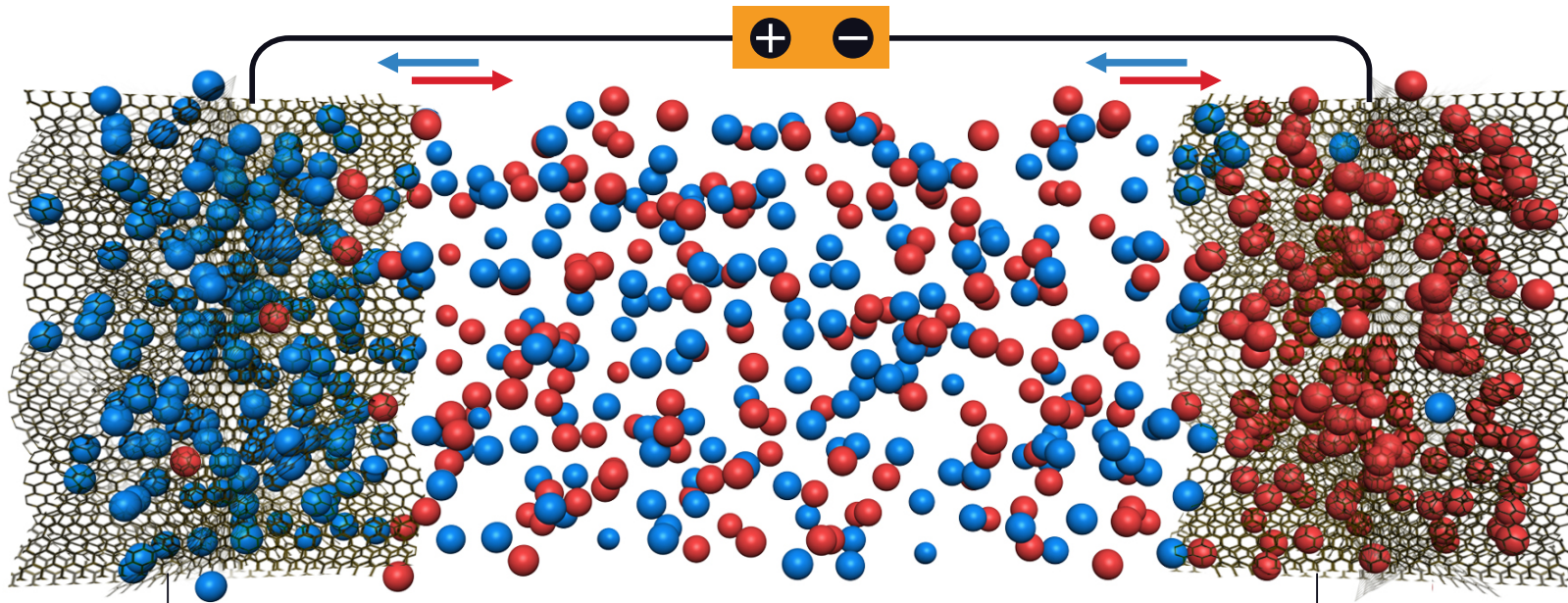
Équilibres redox



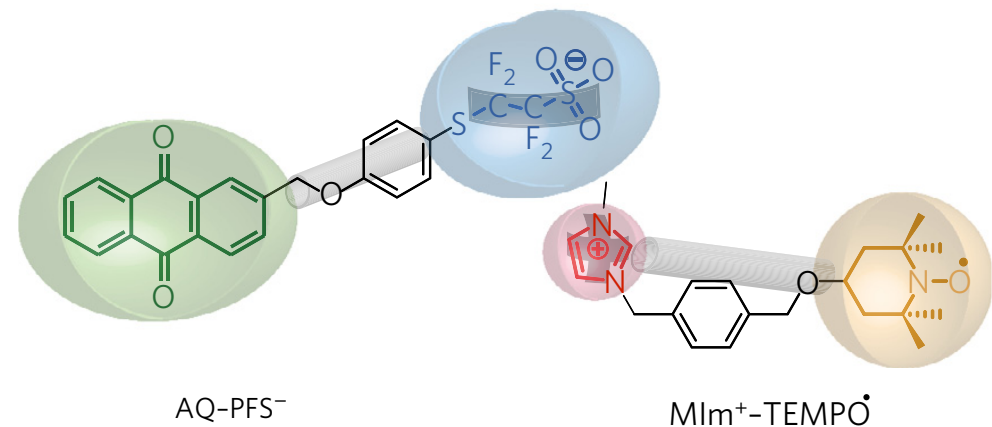
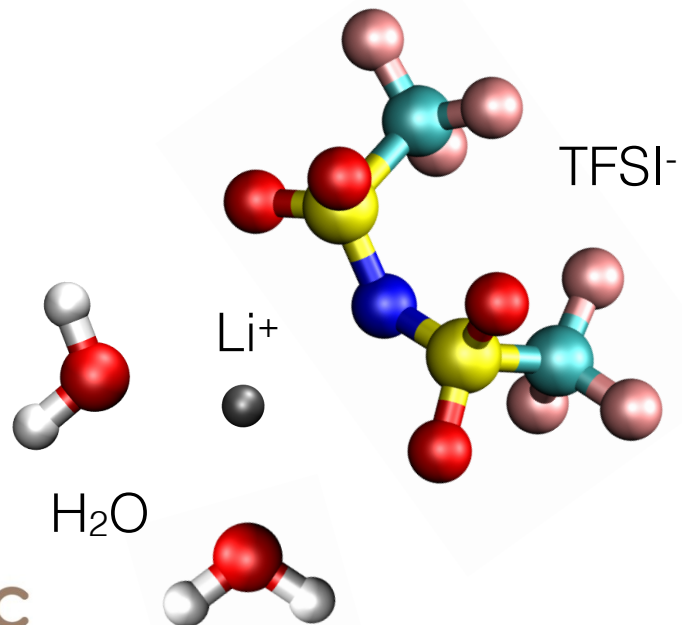
Effet du confinement (thèse Z. Li)



Conclusions & perspectives



La Recherche,
491, 52 (2014)



Remerciements



C. Péan



C. Merlet



B. Rotenberg



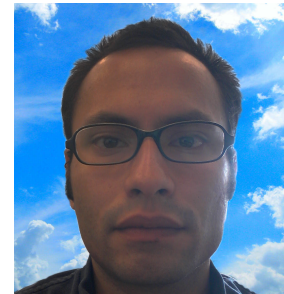
G. Jeanmairét



M. Haefele



T. Mendez



M. Burbano



Z. Li



P. Simon



P. Madden