On the applications of *ab initio* molecular dynamics to enigmatic materials

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In this talk, I will discuss results of ab initio molecular dynamics simulations of complex, disordered systems, including nano-composites of possible use for solar energy conversion [1] and carbon and water in the deep Earth [2].

[1] S.Wippermann et al. *Phys. Rev.Lett.* 110, 046804, (2013); T.Li, F.Gygi and G.Galli, *Phys. Rev. Lett.* 107, 206805 (2011).
[2] L.Spanu et al. *Proc. Nat'l Acd. Sci.* 108, 6843 (2011); D.Pan et al. *Proc. Nat'l Acd.* 2013 (submitted).