

Antonino Marco SAITTA

Grade : Professeur ICL des Universités à l'Université Pierre et Marie Curie
Directeur-Adjoint de la Faculté de Physique de l'Université Pierre et Marie Curie

Section CNU : 28

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie - UMR 7590

Tel : +33.1.44.27.22.44 / Fax : +33.1.44.27.37.85

E-mail : marco.saitta@impmc.upmc.fr

Annexe : Production scientifique

Données bibliométriques générales

- **68 publications** dans revues à comité de lecture, dont :
 - **1 Nature**
 - **2 Nature Materials**
 - **1 PNAS (2014)**
 - **18 Phys. Rev. Lett.**
 - **2 J. Am. Chem. Soc.**
 - **1 Sci. Rep. (2014)**
 - **17 Phys. Rev. B**
 - **2 Phys. Rev. E (Rapid Comm.)**
- **2300+** citations
- **Web of Science h-index = 25**

Publications dans revues internationales à comité de lecture

1. **A.M. Saitta** and F. Saija, *Miller experiments in atomistic computer simulations*, PNAS, **111**, xxxx (2014).
2. Z. Raza, I. Errea, A.R. Oganov, and **A.M. Saitta**, *Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations*, Sci. Rep., **4**, 5889 (2014).
3. Y. Bronstein, Ph. Depondt, F. Finocchi, and **A.M. Saitta** *Quantum-driven phase transition in ice described via an efficient Langevin approach*, Phys. Rev. B, **89**, 214101 (2014).
4. S. Ninet, F. Datchi, et al., and **A.M. Saitta** *Experimental and theoretical evidence for an ionic crystal of ammonia at high pressure*, Phys. Rev. B, **89**, 174103 (2014).
5. G. Cassone, P.V. Giaquinta, F. Saija, and **A.M. Saitta**, *Proton Conduction in Water Ices under an Electric Field*, J. Phys. Chem. B, **118**, 4419 (2014).
6. M. Dagrada, M. Casula, S. Sorella, **A.M. Saitta**, and F. Mauri, *Quantum Monte Carlo study of the protonated water dimer*, J. Chem. Theory Comp., **10**, 1980 (2014).
7. Z. Raza, C.J. Pickard, C. Pinilla, and **A.M. Saitta**, *High Energy Density Mixed Polymeric Phase from Carbon Monoxide and Nitrogen*, Phys. Rev. Lett., **111**, 235501 (2013).
8. L.E. Bove, S. Klotz, Th. Strässle, M. Koza, J. Teixeira, and **A.M. Saitta**, *Translational and Rotational Diffusion in Water in the Gigapascal Range*, Phys. Rev. Lett., **111**, 185901 (2013).
9. **A.M. Saitta**, F. Saija, and P.V. Giaquinta, *Ab Initio Molecular Dynamics Study of Dissociation of Water under an Electric Field*, Phys. Rev. Lett., **108**, 207801 (2012).
10. S. Ninet, F. Datchi, and **A.M. Saitta** *Proton disorder and superionicity in ammonia ice*, Phys. Rev. Lett., **108**, 165702 (2012).
11. R. Jonchière, A.P. Seitsonen, G. Ferlat, **A.M. Saitta**, and R. Vuilleumier, *Van der Waals effects in ab initio water at ambient and supercritical conditions*, J. Chem. Phys. **135**, 154503 (2011).

12. A. Reserbat-Plantey, P. Gava, N. Bendiab, and **A.M. Saitta**, *First principles study of iron-based molecule grafted on graphene*, Europhys. Lett. **96**, 57001 (2011).
13. D. Ziegler et al., *Variations in the work function of doped single- and few-layer graphene assessed by Kelvin probe force microscopy and density functional theory*, Phys. Rev. B **83**, 235434 (2011).
14. L.E. Bove, S. Klotz, J. Philippe, and **A.M. Saitta**, *Pressure-induced polyamorphism of salty water*, Phys. Rev. Lett. **106**, 125701 (2011).
15. A.P. Seitsonen, **A.M. Saitta**, T. Wassmann, M. Lazzeri, F. Mauri, *Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia*, Phys. Rev. B **82**, 115425 (2010).
16. T. Wassmann, A.P. Seitsonen, **A.M. Saitta**, M. Lazzeri, and F. Mauri, *Clar's Theory, π -Electron Distribution, and Geometry of Graphene Nanoribbons*, J. Am. Chem. Soc. **132**, 3440 (2010).
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