

Full list of scientific publications

1. *Inner-Shell Excitation of Gas Phase Carbonates and α,γ -dicarbonyl Compounds*
R. Lessard, **J. Cuny**, G. Cooper, A.P. Hitchcock
Chem. Phys. **2007**, 331, 289-303
2. *DFT Calculations of Quadrupolar Solid-State NMR Properties. Some Examples in Solid-State Inorganic Chemistry*
J. Cuny, S. Messaoudi, V. Alonzo, E. Furet, J.-F. Halet, E. Le Fur, S. E. Ashbrook, C. J. Pickard, R. Gautier, L. Le Pollès
J. Comput. Chem. **2008**, 29, 2279-2287
3. *Redetermination of $Zn_2Mo_3O_8$*
J. Cuny, P. Gougeon, P. Gall
Acta Cryst. **2009**, E65, i51
4. *Synthesis, Electronic and Crystal Structures, and Physical Studies of the Superconductor $Cs_{-1}Mo_{12}S_{14}$, Final Step of the Condensation of the $Mo_6L_8L_6^a$ Unit*
P. Gougeon, D. Salloum, **J. Cuny**, L. Le Pollès, M. Le Floch, R. Gautier, M. Potel
Inorg. Chem. **2009**, 48, 8337-8341
5. *Density Functional Theory Calculations of ^{95}Mo NMR Parameters in Solid-State Compounds*
J. Cuny, E. Furet, R. Gautier, L. Le Pollès, C. J. Pickard, J.-B. d'Espinose de Lacaillerie
ChemPhysChem. **2009**, 10, 3320-3329
6. *Improving Sensitivity and Resolution of MQMAS Spectra: A ^{45}Sc Case Study of Scandium Sulphate Pentahydrate*
C. V. Chandran, **J. Cuny**, R. Gautier, L. Le Pollès, C. J. Pickard, T. Bräuniger
J. Magn. Reson. **2010**, 203, 226-235
7. *Electric Field Gradient Calculations in Paramagnetic Compounds Using the PAW Approach. Application to ^{23}Na NMR in Layered Vanadium Phosphates*
J. Cuny, J. R. Yates, R. Gautier, E. Furet, E. Le Fur, L. Le Pollès
Magn. Reson. Chem. **2010**, 48, S171-S175
8. *High-Temperature Experimental and Theoretical Study of Magnetic Interactions in Diamond and Pseudo-Diamond Frameworks Built up from Hexanuclear Tantalum Clusters*
B. Peric, S. Cordier, **J. Cuny**, R. Gautier, T. Guizouarn, P. Planinic
Chem.--Eur. J. **2011**, 17, 6263
9. *^{95}Mo nuclear magnetic resonance parameters of molybdenum hexacarbonyl from density functional theory: appraisal of computational and geometrical parameters*
J. Cuny, K. Sykina, B. Fontaine, L. Le Pollès, C. J. Pickard, R. Gautier
Phys. Chem. Chem. Phys. **2011**, 13, 19471-19479
10. *Exploring the free energy surfaces of clusters using reconnaissance metadynamics*
G. A. Tribello, **J. Cuny**, H. Eshet, M. Parrinello
J. Chem. Phys. **2011**, 135, 114109
11. *Synthesis, Crystal and Electronic Structures, and Magnetic Properties of the $LiLn_9Mo_{16}O_{35}$ ($Ln = La, Ce, Pr, \text{ and } Nd$) Compounds Containing the Original Cluster $Mo_{16}O_{36}$.*
P. Gougeon, P. Gall, **J. Cuny**, R. Gautier, L. Le Pollès, L. Delevoye, J. Trèbosc
Chem.--Eur. J. **2011**, 17, 13806-13813

12. *The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates*
A. A. Hassanali, **J. Cuny**, M. Ceriotti, C. J. Pickard, M. Parrinello
J. Am. Chem. Soc. **2012**, *134*, 8557-8569
13. *⁹⁵Mo Solid-State Nuclear Magnetic Resonance Spectroscopy and Quantum Simulations : Synergetic Tools for the Study of Molybdenum Cluster Materials*
J. Cuny, S. Cordier, C. Perrin, C. J. Pickard, L. Delevoye, J. Trèbosc, Z. Gan, L. Le Pollès, R. Gautier
Inorg. Chem. **2013**, *52*, 617-627
14. *Synthesis, crystal and electronic structures and magnetic properties of Li₂SnMo₃O₈:A novel reduced molybdenum oxide containing Mo₃O₁₃ cluster units*
P. Gall, R. Al Rahal Al Orabi, T. Guizouarn, **J. Cuny**, B. Fontaine, R. Gautier, P. Gougeon
J. Solid State Chem. **2013**, *201*, 312-316
15. *Shape Modulation of Octanuclear Cu(I) or Ag(I) Dichalcogeno Template Clusters with Respect to the Nature of their Encapsulated Anions: A Combined Theoretical and Experimental Investigation*
C. Latouche, S. Kahlal, E. Furet, P.-K. Liao, Y.-R. Lin, C.-S. Fang, **J. Cuny**, C. W. Liu, J.-Y. Saillard
Inorg. Chem. **2013**, *52*, 617-627
16. *Proton transfer through the water gossamer*
A. A. Hassanali, F. Giberti, **J. Cuny**, T. D. Kühne, M. Parrinello
PNAS **2013**, *110*, 13723-13728
17. *Nuclear quantum effects and hydrogen bond fluctuations in water*
M. Ceriotti, **J. Cuny**, M. Parrinello, D. E. Manolopoulos
PNAS **2013**, *110*, 15591-15596
18. *Aqueous solutions: state of the art in ab initio molecular dynamics*
A. A. Hassanali, **J. Cuny**, V. Verdolino, M. Parrinello
Phil. Trans. R. Soc. A **2014**, *372*, 20120482
19. *Ab Initio Molecular Dynamics Study of the Mechanism of Proton Recombination with a Weak Base*
J. Cuny and A. A. Hassanali
J. Phys. Chem. B **2014**, *118*, 13903-13912
20. *Phase changes of the water hexamer and octamer in the gas phase and adsorbed on polycyclic aromatic hydrocarbons*
L. F. L. Oliveira, **J. Cuny**, M. Morinière, L. Dontot, A. Simon, F. Spiegelman, M. Rapacioli
Phys. Chem. Chem. Phys. **2015**, *17*, 17079-17089
21. *Evaluation of ⁹⁵Mo Nuclear Shielding and Chemical Shift of [Mo₆X₁₄]²⁻ Clusters in the Liquid Phase*
T. T. Nguyen, J. Jung, X. Trivelli, J. Trèbosc, S. Cordier, Y. Molard, L. LePollès, C. J. Pickard, **J. Cuny**, R. Gautier
Inorg. Chem. **2015**, *54*, 7673-7683
22. *Combined theoretical and time-resolved photoluminescence investigations of [Mo₆Br₈Br₆]²⁻ metal cluster units: evidences of dual emission*
K. Costuas, A. Garreau, A. Bulou, B. Fontaine, **J. Cuny**, R. Gautier, M. Mortier, Y. Molard, J.-L. Duvail, E. Faulques, S. Cordier
Phys. Chem. Chem. Phys. **2015**, *17*, 28574
23. *Cationic Methylene-Pyrene Isomers and Isomerization Pathways: Finite Temperature Theoretical Studies*
M. Rapacioli, A. Simon, C. Marshall, **J. Cuny**, D. Kokkin, F. Spiegelman, C. Joblin
J. Phys. Chem. A **2015**, *119*, 12845-12854
24. *Ab Initio Quality NMR Parameters in Solid-State Materials Using a High-Dimensional Neural-Network*

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- J. Cuny**, Y. Xie, C. J. Pickard, and A. A. Hassanali
J. Chem. Theory Comput. **2016**, 12 (2), 765–773
25. *Benchmarking DFTB for Silver and Gold Materials: From Small Clusters to Bulk*
L. F. L. Oliveira, N. Tarrat, **J. Cuny**, J. Morillo, D. Lemoine, F. Spiegelman, M. Rapacioli
J. Phys. Chem. A **2016**, 120, 8469-8483
26. *Structural Characterisation of Sulfur-Containing Water Clusters Using a Density-Functional Based Tight-Binding Approach*
K. A. Korchagina, A. Simon, M. Rapacioli, F. Spiegelman, **J. Cuny**
J. Phys. Chem. A **2016**, 120, 9089-9100
27. *Keto-polymethines: a versatile class of dyes with outstanding spectroscopic properties for in cellulose and in vivo two-photon microscopy imaging*
S. Pascal, S. Denis-Quanquin, F. Appaix, A. Duperray, A. Grichine, B. Le Guennic, D. Jacquemin, **J. Cuny**, S.-H. Chi, J. W. Perry, B. van der Sanden, C. Monnereau, C. Andraud, O. Maury
Chem. Sci. **2017**, 8, 381-394
28. *Metadynamics combined with Auxiliary Density Functional and Density Functional Tight Binding Methods: Alanine Dipeptide as a Case Study*
J. Cuny, K. Korchagina, C. Menakbi T. Mineva
J. Mol. Model., **2017**, 23, 71
29. *Global Optimization of Neutral and Charged 20- and 55-Atom Silver and Gold Clusters at the DFTB Level*
N. Tarrat, M. Rapacioli, **J. Cuny**, J. Morillo, F. Spiegelman
Comp. Theor. Chem., **2017**, 1107, 102-114
30. *Pesticide interaction with environmentally important cations: A molecular dynamics and DFT study of metamitron and fenhexamid*
B. Belzunces, S. Hoyau, **J. Cuny**, F. Bessac
Comp. Theor. Chem., **2017**, 1117, 220-234.
31. *Theoretical Investigation of the Solid-Liquid Phase Transition in Protonated Water Clusters*
K. Korchagina, A. Simon, M. Rapacioli, F. Spiegelman, J.-M. L'Hermite, I Braud, S. Zamith, **J. Cuny**
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32. *Molecular Dynamics Study of the Collision-Induced Reaction of H with CO on Small Water Clusters*
K. Korchagina, F. Spiegelman, **J. Cuny**
J. Phys. Chem. A, **2017**, 121, 9485-9494.
33. *Conformational Study and Chiroptical Properties of Chiral Dimethyl- Ethylenedithio-Tetrathiafulvalene (DM-EDT-TTF)*
T. Cauchy, F. Pop, **J. Cuny**, N. Avarvari
Chimia, **2018**, 72, 1-5.
34. *Density-functional tight-binding approach for metal clusters, nanoparticles, surfaces and bulk: application to silver and gold*
J. Cuny, N. Tarrat, F. Spiegelman, A. Huguenot, A. Rapacioli
J. Phys.: Condens. Matter, **2018**, 30, 30.
35. *Metal Atom Clusters as Building Blocks for Multifunctional Proton-Conducting Materials: Theoretical and Experimental Characterization*
G. Daigre, **J. Cuny**, P. Lemoine, M. Amela-Cortes, S. Paofai, N. Audebrand, A. Le Gal La Salle, E. Quarez, O. Joubert, N. G. Naumov, S. Cordier

Inorg. Chem., **2018**, *57*, 9814–9825

36. *Evaluation of Gas-to-Liquid ¹⁷O Chemical Shift of Water: A Test Case for Molecular and Periodic Approaches*
J. Cuny, F. Jolibois, I. C. Gerber
J. Chem. Theory Comput., **2018**, *14*, 4041-4051
37. *Selective assembly of Molybdenum Clusters into Nanomarbles and Nanocapsules*
F. Sciortino, J. Cuny, F. Grasset, C. Lagrost, P. Lemoine, A. Moréac, Y. Molard, T. Takei, S. Cordier, S. Chevance, F. Gauffre
ChemComm, **2018**, *54*, 13387-13390.
38. *Contribution of the Density-Functional based Tight-Binding Scheme to the Description of Water Clusters : Methods, Applications and Extension to Bulk Systems*
A. Simon, M. Rapacioli, E. Michoulier, L. Zheng, K. Korchagina, J. Cuny
Mol. Sim., **2019**, *45*, 249-268
39. *Size-Dependent Proton Localization in Hydrated Uracil Clusters: A Joint Experimental and Theoretical Study*
I. Braud, S. Zamith, J. Cuny, L. Zheng, J.-M. L'Hermite
J. Chem. Phys., **2019**, *150*, 014303
40. A. de la Lande, A. Alvarez-Ibarra, K. Hasnaoui, F. Cailliez, X. Wu, T. Mineva, J. Cuny, P. Calaminici, L. López-Sosa, G. Geudtner, I. Navizet, C. G. Iriepa, D. R. Salahub, A. M. Köster
Molecules, **2019**, *24*, 1653

Complete List of Book Chapters

1. First-Principles Computation of NMR Parameters in Solid-State Chemistry. In *Handbook of Solid State Chemistry* (eds R. Dronskowski, S. Kikkawa and A. Stein). **2017**
J. Cuny, R. Gautier, J.-F. Halet