

## Liste de publications de Rodolphe Vuilleumier

### 1. Articles dans des journaux à comités de lecture

- [1] Sanctis, Maria ; Politis, marie ; Vuilleumier, Rodolphe ; Stia, C ; Fojon, Omar *Theoretical study of the ionization of liquid water from its several initial orbitals by fast electron impact* accepté à Journal of Physics B : Atomic, Molecular and Optical Physics.
- [2] Pinilla, Carlos, Marc Blanchard, Etienne Balan, Suresh K. Natarajan, Rodolphe Vuilleumier, et Francesco Mauri. *Equilibrium magnesium isotope fractionation between aqueous Mg<sup>2+</sup> and carbonate minerals : Insights from path integral molecular dynamics*. In press at Geochimica et Cosmochimica Acta. doi:10.1016/j.gca.2015.04.008 (2015).
- [3] Morizet, Y., R. Vuilleumier, et M. Paris. *A NMR and molecular dynamics study of CO<sub>2</sub>-bearing basaltic melts and glasses*. In press at Chemical Geology. doi:10.1016/j.chemgeo.2015.03.021 (2015).
- [4] Vuilleumier, Rodolphe, Ari P. Seitsonen, Nicolas Sator, et Bertrand Guillot. *Carbon dioxide in silicate melts at upper mantle conditions : Insights from atomistic simulations* In press at Chemical Geology. doi:10.1016/j.chemgeo.2015.02.027 (2015).
- [5] Agostini, F., Ciccotti, G., Savin, A. and Vuilleumier, R. *Maximum probability domains for the analysis of the microscopic structure of liquids*. The Journal of Chemical Physics 142, 064117 (2015).
- [6] Vuilleumier, R., Seitsonen, A., Sator, N. and Guillot, B. *Structure, equation of state and transport properties of molten calcium carbonate (CaCO<sub>3</sub>) by atomistic simulations*. Geochimica et Cosmochimica Acta 141, 547-566 (2014).
- [7] Beutier, J., Borgis, D., Vuilleumier, R. and Bonella, S. *Computing thermal Wigner densities with the phase integration method*. The Journal of Chemical Physics 141, 084102 (2014).
- [8] Haigis, V., Belkhodja, Y., Coudert, F.-X., Vuilleumier, R. and Boutin, A. *Challenges in first-principles NPT molecular dynamics of soft porous crystals : A case study on MIL-53(Ga)*. The Journal of Chemical Physics 141, 064703 (2014).
- [9] Spezia, R., Jeanvoine, Y. and Vuilleumier, R. *Developing polarizable potential for molecular dynamics of Cm(III)-carbonate complexes in liquid water*. J Mol Model 20, 1-9 (2014).
- [10] Lasoroski, A., Vuilleumier, R. and Pollet, R. *Vibrational dynamics of zero-field-splitting hamiltonian in gadolinium-based MRI contrast agents from ab initio molecular dynamics*. The Journal of Chemical Physics 141, 014201 (2014).
- [11] Pinilla, C., Blanchard, M., Balan, E., Ferlat, G., Vuilleumier, R. and Mauri, F. *Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics*. Geochimica et Cosmochimica Acta 135, 203-216 (2014).
- [12] Vuilleumier, R. *Atomic partial charges in condensed phase from an exact sum rule for infrared absorption*. Molecular Physics 112, 1457-1462 (2014).
- [13] Kish, E., Mendes Pinto, M. M., Bovi, D., Basire, M., Guidoni, L., Vuilleumier, R., Robert, B., Spezia, R. and Mezzetti, A. *Fermi Resonance as a Tool for Probing Peridinin Environment*. J. Phys. Chem. B 118, 5873-5881 (2014).
- [14] Penhoat, M. A. H., López-Tarifa, P., Ghose, K. K., Jeanvoine, Y., Gageot, M.-P., Vuilleumier, R., Politis, M.-F. and Bacchus-Montabonel, M.-C. *Modeling proton-induced damage on 2-deoxy-D-ribose. Conformational analysis*. J Mol Model 20, 1-8 (2014).

- [15] Carof, A., Vuilleumier, R. and Rotenberg, B. *Two algorithms to compute projected correlation functions in molecular dynamics simulations*. The Journal of Chemical Physics 140, 124103 (2014).
- [16] Spezia, R., Jeanvoine, Y., Beuchat, C., Gagliardi, L. and Vuilleumier, R. *Hydration properties of Cm(III) and Th(IV) combining coordination free energy profiles with electronic structure analysis*. Phys. Chem. Chem. Phys. 16, 5824–5832 (2014).
- [17] Martelli, F. Jeanvoine, Y., Vercouter, T., Beuchat, C., Vuilleumier, R. and Spezia, R. *Hydration properties of lanthanoid(III) carbonate complexes in liquid water determined by polarizable molecular dynamics simulations*. Phys. Chem. Chem. Phys. 16, 3693–3705 (2014).
- [18] López-Tarifa, P., Hervé du Penhoat, M.-A., Vuilleumier, R., Gaigeot, M.-P., Rothlisberger, U., Tavernelli, I., Le Padellec, A., Champeaux, J.-P., Alcamí, M., Moretto-Capelle, P., Martin, F. and Politis, M.-F. *Time-dependent density functional theory molecular dynamics simulation of doubly charged uracil in gas phase*. centr.eur.j.phys. 12, 97–102 (2014).
- [19] Beutier, J., Monteferrante, M., Bonella, S., Vuilleumier, R. and Ciccotti, G. *Gas phase infrared spectra via the phase integration quasi-classical method*. Molecular Simulation 40, 196–207 (2014).
- [20] Arne Scherrer, Rodolphe Vuilleumier, Daniel Sebastiani, *Nuclear Velocity Perturbation Theory of Vibrational Circular Dichroism*, J. Chem. Theory Comput. 9, 5305 (2013).
- [21] Aurélie Lasoroski, Rodolphe Vuilleumier, Rodolphe Pollet, *Hyperfine interactions in a gadolinium-based MRI contrast agent : High-frequency modulations from ab initio simulations*, J. Chem. Phys. 139, 104115 (2013)
- [22] Mayeul Collot, Aurélie Lasoroski, Alsu I. Zamaleeva, Anne Feltz, Rodolphe Vuilleumier, Jean-Maurice Mallet, *Unexpected remote effect in red fluorescent sensors based on extended APTRA* Tetrahedron 69, 10482-10487 (2013).
- [23] Julien Beutier, Michele Monteferrante, Sara Bonella, Rodolphe Vuilleumier, Giovanni Ciccotti, *Gas phase infrared spectra via the phase integration quasi-classical method*, Mol. Sim. 40, 196-207 (2013).
- [24] Riccardo Spezia, Rodolphe Vuilleumier, *Computation of pair distribution functions and three-dimensional densities with a reduced variance principle*, Mol. Phys. 111, 3478 (2013).
- [25] Daniel Borgis, Rolland Assaraf, Benjamin Rotenberg, Rodolphe Vuilleumier, *Computation of pair distribution functions and three-dimensional densities with a reduced variance principle*, Mol. Phys. 111, 3486 (2013).
- [26] Volker Haigis, François-Xavier Coudert, Rodolphe Vuilleumier, Anne Boutin, *Investigation of structure and dynamics of the hydrated metal-organic framework MIL-53(Cr) using first-principles molecular dynamics*, PCCP 15, 19049-19056 (2013).
- [27] Marie Basire, Daniel Borgis, Rodolphe Vuilleumier, *Computing Wigner distributions and time correlation functions using the quantum thermal bath method : application to proton transfer spectroscopy*, PCCP 15, 12591-12601 (2013).
- [28] Pablo López-Tarifa, Marie-Pierre Gaigeot, Rodolphe Vuilleumier, Ivano Tavernelli, Manuel Alcamí, Fernando Martín, Marie-Anne Hervé du Penhoat and Marie-Françoise Politis, *You have full text access to this content Ultrafast Damage Following Radiation-Induced Oxidation of Uracil in Aqueous Solution*, Angew. Chem. Intl. Ed. 52, 3160 (2013).
- [29] Guillaume Jeanmairet, Maximilien Levesque, Rodolphe Vuilleumier, Daniel Borgis, *Molecular density functional theory of water*, J. Phys. Chem. Lett. 4, 619 (2013).
- [30] Gleb S. Pokrovski, Jacques Roux, Guillaume Ferlat, Romain Jonchiere, Ari P. Seitsonen, Rodolphe Vuilleumier, Jean-Louis Hazemann, *Silver in geological fluids from in situ X-ray*

*absorption spectroscopy and first-principles molecular dynamics*, *Geochimica et Cosmochimica Acta* 106, 501 (2013).

- [31] F. Martelli, S. Abadie, J.-P. Simonin, R. Vuilleumier, R. Spezia, *Lanthanoids(III) and actinoids(III) in water : Diffusion coefficients and hydration enthalpies from polarizable molecular dynamics simulations*, *Pure and applied chemistry* 85, 237 (2013).
- [32] Maximilien Levesque, Virginie Marry, Benjamin Rotenberg, Guillaume Jeanmairret, Rodolphe Vuilleumier et Daniel Borgis, *Solvation of complex surfaces via molecular density functional theory*, *J. Chem. Phys.* 137, 224107 (2012).
- [33] Fausto Martelli, Rodolphe Vuilleumier, Jean-Pierre Simonin, and Riccardo Spezia, *Varying the charge of small cations in liquid water : Structural, transport, and thermodynamical properties*, *J. Chem. Phys.* 137, 164501 (2012)
- [34] Maximilien Levesque, Rodolphe Vuilleumier, Daniel Borgis, *Scalar fundamental measure theory for hard spheres in three dimensions : Application to hydrophobic solvation*, *J. Chem. Phys.* 137, 034115 (2012).
- [35] Riccardo Spezia, Cesar Beuchat, Rodolphe Vuilleumier, Paola D’Angelo, and Laura Gagliardi, *Unravelling the Hydration Structure of ThX<sub>4</sub> (X = Br, Cl) Water Solutions by Molecular Dynamics Simulations and X-ray Absorption Spectroscopy* *J. Phys. Chem. B* 116, 6465–6475 (2012)
- [36] S. Tazi, J. J. Molina, B. Rotenberg, P. Turq, R. Vuilleumier and M. Salanne, *A transferable ab initio based force field for aqueous ions*, *Journal of Chemical Physics* 136, 114507 (2012)
- [37] Rodolphe Vuilleumier, Daniel borgis, *Proton Conduction – Hopping along hydrogen bonds*, *Nature Chemistry* 4, 432-433, [doi:10.1038/nchem.1365](https://doi.org/10.1038/nchem.1365) .
- [38] M.-L. de Sanctis, M.F. Politis, R. Vuilleumier, C. R. Stia, O. A. Fojon, *Liquid water ionization by fast electron impact : a multiple differential study for the 1B 1 orbital*. *Journal of Physics B : Atomic, Molecular and Optical Physics* 45, 045206 (2012).
- [39] M. Salanne, B. Rotenberg, S. Jahn, R. Vuilleumier, C. Simon and P. Madden, *Including many-body effects in models for ionic liquids*. *Theoretical Chemistry Accounts : Theory, Computation, and Modeling (Theoretica Chimica Acta)* 131, 1143 (2012).
- [40] R. Vuilleumier, K. Tay, G. Jeanmairret, D. Borgis and A. Boutin, *Extension of Marcus picture for electron transfer reactions with large solvation changes*, *J. Am. Chem. Soc.* 134, 2067-2074 (2011), [doi:10.1021/ja2069104](https://doi.org/10.1021/ja2069104) .
- [41] D. Bovi, A. Mezzetti, R. Vuilleumier, M.-P. Gageot, B. Chazallon, R. Spezia and L. Guidoni *Environmental effects on vibrational properties of carotenoids : experiments and calculations on peridinin*, *Phys. Chem. Chem. Phys.* 13, 20954 (2011), [doi:10.1039/C1CP21985E](https://doi.org/10.1039/C1CP21985E) .
- [42] 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), [doi:10.1063/1.3651474](https://doi.org/10.1063/1.3651474)
- [43] P. Lopez-Tarifa, M.-A. Hervé du Penhoat, R. Vuilleumier, M.-P. Gageot, I. Tavernelli, A. Le Padellec, J.-P. Champeaux, M. Alcami, P. Moretto-Capelle, F. Martin and M.-F. Politis, *Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase*, *Phys. Rev. Lett.* 107, 023202 (2011), [doi:10.1103/PhysRevLett.107.023202](https://doi.org/10.1103/PhysRevLett.107.023202) .
- [44] S. Zhao, R. Ramirez, R. Vuilleumier, and D. Borgis, *Molecular Density Functional Theory of Solvation : From polar solvents to water* , *J. Chem. Phys.* **134**, 194102 (2011), [doi:10.1063/1.3589142](https://doi.org/10.1063/1.3589142)
- [45] R. Vuilleumier, N. Sator and B. Guillot, *Electronic redistribution around oxygen atoms in silicate melts by ab initio molecular dynamics simulation*, *Journal of Non-Crystalline Solids* **357**, 2555 (2011), [doi:10.1016/j.jnoncrysol.2011.02.051](https://doi.org/10.1016/j.jnoncrysol.2011.02.051) .

- [46] R. Spezia, B. Siboulet, S. Abadie, R. Vuilleumier and P. Vitorge, *Stability and Instability of the Isoelectronic  $UO_2^{2+}$  and  $PaO_2^+$  Actinyl Oxo-Cations in Aqueous Solution from Density Functional Theory Based Molecular Dynamics*, J. Phys. Chem. B **115**, 3560 (2011), doi: [10.1021/jp111726b](https://doi.org/10.1021/jp111726b) .
- [47] F. Agostini, R. Vuilleumier and G. Ciccotti, *Infrared spectroscopy of small protonated water clusters at room temperature : an effective modes analysis*, J. Chem. Phys. **134**, 084301 (2011)
- [48] F. Agostini, R. Vuilleumier and G. Ciccotti, *Infrared spectroscopy and effective modes analysis of the protonated water dimer  $H^+(H_2O)_2$  at room temperature under H/D substitution*, J. Chem. Phys. **134**, 084302 (2011)
- [49] A. Jezierska-Mazzarello, J. J. Panek, R. Vuilleumier, A. Koll and G. Ciccotti, *Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff bases-A comparative molecular dynamics study*, J. Chem. Phys. **134**, 034308 (2011).
- [50] C. R. Stia, M.-P. Gaigeot, R. Vuilleumier, O. A. Fojon, M.-A. Hervé du Penhoat, M.-F. Politis, *Theoretical investigation of the ultrafast dissociation of core-ionized water and uracil molecules immersed in liquid water*, Eur. Phys. J. D **60**, 77 (2010)
- [51] R. Ayala, R. Spezia, R. Vuilleumier, J. M. Martinez, R. R. Pappalardo and E. Sanchez Marcos, *An Ab Initio Molecular Dynamics Study on the Hydrolysis of the Po(IV) Aquaion in Water*, J. Phys. Chem. B **114**, 12866 (2010).
- [52] C. Terrier, P. Vitorge, M.-P. Gaigeot, R. Spezia and R. Vuilleumier, *Density functional theory based molecular dynamics study of hydration and electronic properties of aqueous  $La^{3+}$* , J. Chem. Phys. **133**, 044509 (2010).
- [53] M.-P. Gaigeot, P. Lopez-Tarifa, F. Martin, M. Alcamí, R. Vuilleumier, I. Tavernelli, M.-A. Hervé du Penhoat, M.-F. Politis, *Theoretical investigation of the ultrafast dissociation of ionized biomolecules immersed in water : Direct and indirect effects*, Mutation Research-Reviews in Mutation Research **704**, 45 (2010).
- [54] B. Rotenberg, M. Salanne, C. Simon and R. Vuilleumier, *From Localized Orbitals to Material Properties : Building Classical Force Fields for Nonmetallic Condensed Matter Systems*, Phys. Rev. Lett. **104**, 138101 (2010).
- [55] A. Jezierska-Mazzarello, R. Vuilleumier, J. Panek and G. Ciccotti. *Molecular Property Investigations of an ortho-hydroxy Schiff base type compound with First-Principle Molecular Dynamics approach*, J. Phys. Chem. B. **114**, 242 (2010).
- [56] R. Vuilleumier, N. Sator and B. Guillot *Computer modeling of natural silicate melts : what can we learn from ab initio simulations*, Geochemica and Cosmochimica Acta **73**, 6313 (2009).
- [57] M. Micoulaut, R. Vuilleumier and C. Massobrio *Improved modeling of liquid  $GeSe_2$  : Impact of the exchange-correlation functional*, Phys. Rev. B **79**, 214205 (2009).
- [58] L. Adoui, A. Cassimi, B. Gervais, J.-P. Grandin, L. Guillaume, R. Maisonnay, S. Legendre, M. Taxisien, P. Lopez-Tarifa, M.-F. Politis, M.-A. Herve du Penhoat, R. Vuilleumier, M.-P. Gaigeot, I. Tavernelli, M. Alcamí and F. Martin, *Ionization and fragmentation of water clusters by fast highly charged ions*, J. Phys. B **42**, 075101 (2009).
- [59] F.-X. Coudert, F. Cailliez, R. Vuilleumier, A. H. Fuchs and A. Boutin *Water nanodroplets confined in zeolite pores*, Faraday Discuss. **141**, 377 (2009).
- [60] M. Salanne, R. Vuilleumier, P. A Madden, C. Simon, P. Turq, B. Guillot, *Polarizabilities of individual molecules and ions in liquids from first-principles*, J. Phys. : Condens. Matter **20**, 494207 (2008).
- [61] X. Rozanska, R. Vuilleumier *Mechanisms of the Water-Gas-Shift Reaction by Iron Pentacarbonyl in the Gas Phase* Inorg. Chem. **47**, 8635 (2008).

- [62] I. Tavernelli, M.-P. Gaigeot, R. Vuilleumier, C. Stia, M.-A. Hervé du Penhoat, M.-F. Politis *Time-Dependent Density Functional Theory Molecular Dynamics Simulations of Liquid Water Radiolysis*, ChemPhysChem **9**, 2099 (2008)
- [63] L. Petit, R. Vuilleumier, P. Maldivi, C. Adamo *Molecular dynamics study of the coordination sphere of trivalent lanthanum in a highly concentrated LiCl aqueous solution : A combined classical and ab initio approach* J. Phys. Chem. B. **112**, 10603 (2008).
- [64] J.-P. Renault, R. Vuilleumier, S. Pommeret *Hydrated electron production by reaction of hydrogen atoms with hydroxide ions : a first principle molecular dynamics study* J. Phys. Chem. A. **112**, 7027 (2008).
- [65] L. Petit, R. Vuilleumier, P. Maldivi, C. Adamo *Ab initio molecular dynamics study of a highly concentrated LiCl aqueous solution*, J. Chem. Theo. Comp. **4**, 1040 (2008).
- [66] M.P. Gaigeot, R. Vuilleumier, M. Martinez *Infrared spectroscopy in the gas and liquid phase from first principle molecular dynamics simulations – Application to small peptides* Molecular Physics **105**, 2857 (2007).
- [67] B. Rotenberg, V. Marry, R. Vuilleumier, et al. *Water and ions in clays : Unraveling the interlayer/micropore exchange using molecular dynamics* Geochimica and Cosmochimica Acta **71**, 5089 (2007).
- [68] Wafa Amir, Guilhem Gallot, Francois Hache, S. Bratos, J.-C. Leicknam, et R. Vuilleumier, *Time-resolved observation of the Eigen cation in liquid water* J. Chem. Phys. **126**, 034511 (2007).
- [69] M.P. Gaigeot, R. Vuilleumier, C. Stia, M.E. Galassi, R. Rivarola, B. Gervais, M.F. Politis, *A multi-scale ab initio theoretical study of the production of free radicals in swift ion tracks in liquid water*, J. Phys. B : At. Mol. Opt. Phys. **40**, 1 (2007).
- [70] F. X. Coudert, R. Vuilleumier et A. Boutin, *Dipole moment, hydrogen bonding and IR spectrum of confined water*, ChemPhysChem **7**, 2464 (2006).
- [71] M. Martinez, M.-P. Gaigeot, D. Borgis et R. Vuilleumier *Extracting effective normal modes from equilibrium dynamics at finite temperature*, Journal of Chemical Physics **125**, 144106 (2006).
- [72] Q. Y. Kong, M. Wulff, S. Bratos, R. Vuilleumier, J. Kim et H. Ihee *Structure of the photodissociation products of CCl<sub>4</sub>, CBr<sub>4</sub>, and CI<sub>4</sub> in solution studied by DFT and ab initio calculations*, Journal of Physical Chemistry A **110** (38), 11178 (2006).
- [73] M.S. Causo, G. Ciccotti, S. Bonella et R. Vuilleumier *An adiabatic linearized path integral approach for quantum time-correlation functions II : A cumulant expansion method for improving convergence*, Journal of Physical Chemistry B **110**, 16026 (2006).
- [74] G. Kalibaeva, R. Vuilleumier, S. Meloni, A. Alavi, G. Ciccotti et R. Rosei *Ab Initio simulation of carbon clustering on Ni(111) surface : a model of the poisoning of nickel catalysts* Journal of Physical Chemistry B **110**, 3638 (2006).
- [75] M. Wulff, S. Bratos, A. Plech, R. Vuilleumier, F. Mirloup, M. Lorenc, Q. Kong et H. Ihee *Recombination of Photo-Dissociated Iodine : a Time-Resolved x-Ray Diffraction Study* Journal of Chemical Physics **124**, 034501 (2006).
- [76] B. Cabane et R. Vuilleumier, *The physics of liquid water* Comptes rendus géosciences **337**, 159-171 (2005).
- [77] M. P. Gaigeot, R. Vuilleumier, M. Sprik, et D. Borgis *Infrared Spectroscopy of N-Methylacetamide Revisited by ab Initio Molecular Dynamics Simulations* Journal of Chemical Theory and Computation **1**, 772 (2005).

- [78] L. Bernasconi, J. Blumberger, M. Sprik et R. Vuilleumier *Density functional calculation of the electronic absorption spectrum of  $\text{Cu}^+$  and  $\text{Ag}^+$  aqua ions* Journal of Chemical Physics **121**, 11885 (2004).
- [79] R. Spezia, C. Nicolas, F.-X. Coudert, P. Archirel, R. Vuilleumier and A. Boutin *Reactivity of an excess electron with monovalent cations in bulk water by mixed quantum classical molecular dynamics simulations* Molecular Simulation **30**, 749 (2004).
- [80] F. Mirloup, R. Vuilleumier, M. Wulff, A. Plech and S. Bratos, *X-Ray "Filming" of Atomic Motions in Chemical Reactions*, Chemical Physics **304**, 245 (2004)
- [81] A. Plech, M. Wulff, S. Bratos, F. Mirloup, R. Vuilleumier, F. Schotte, and P. A. Anfinrud *Visualizing Chemical Reactions in Solution by Picosecond X-Ray Diffraction*, Phys. Rev. Lett. **92**, 125505 (2004).
- [82] J. Blumberger, L. Bernasconi, I. Tavernelli, R. Vuilleumier and M. Sprik, *Electronic Structure and Solvation of Copper and Silver Ions : A Theoretical Picture of a Model Aqueous Redox Reaction*, J. Am. Chem. Soc. **126**, 3928 (2004).
- [83] C. Nicolas, R. Spezia, A. Boutin et R. Vuilleumier, *Molecular Dynamics simulations of a silver atom in water : dipolar excitonic state evidence*, Phys. Rev. Lett. **91**, 208304 (2003).
- [84] P. Hunt, M. Sprik et R. Vuilleumier, *Thermal versus electronic broadening in the density of states of liquid water*, Chem. Phys. Lett. **376**, 68 (2003).
- [85] A. Plech, R. Randler, M. Wulff, F. Mirloup and R. Vuilleumier, *Determination of structure in liquid solutions – implications for picosecond photoexcitation studies* Journal of Physics : Condensed Matter, **15**, 2002 (S137).
- [86] R. Vuilleumier and M. Sprik, *Electronic control of reactivity using density functional perturbation methods* Chem. Phys. Lett., **365**, 2002 (305).
- [87] S. Bratos, F. Mirloup, R. Vuilleumier, and M. Wulff, *Time-resolved x-ray diffraction : Statistical theory and its application to the photo-physics of molecular iodine* Journal of Chemical Physics **116**, 2002 (10615).
- [88] I. Tavernelli, R. Vuilleumier and M. Sprik, *Ab Initio Molecular Dynamics for Molecules with Variable Numbers of Electrons* Phys. Rev. Lett. **88**, 2002 (213002).
- [89] R. Vuilleumier and M. Sprik, *Electronic Properties of Hard and Soft Ions in Solution : aqueous  $\text{Na}^+$  and  $\text{Ag}^+$  compared*, Journal of Chemical Physics **115**, 2001 (3454).
- [90] R. Vuilleumier, M. Sprik and A. Alavi, *Computation of Electronic Chemical Potentials using Free Energy Density Functionals*, Journal of Molecular Structure (THEOCHEM) **506**, 2000 (343).
- [91] R. Vuilleumier and D. Borgis, *An Extended Empirical Valence Bond Model for Describing Proton Mobility in Water*, Israel Journal of Chemistry **39**, 1999 (457).
- [92] R. Vuilleumier and D. Borgis, *Wavefunction quantisation of the proton motion in a  $\text{H}_5\text{O}_2^+$  dimer solvated in liquid water*, Journal of Molecular Structure **552**, 2000 (117).
- [93] R. Vuilleumier and D. Borgis, *Transport and spectroscopy of the hydrated proton : A molecular dynamics study*, Journal of Chemical Physics **111**, 1999 (4251).
- [94] X. Krokidis, R. Vuilleumier, D. Borgis and B. Silvi, *Topological analysis of the proton transfer in  $\text{H}_5\text{O}_2^+$* , Molecular Physics **96**, 1999 (265).
- [95] R. Vuilleumier and D. Borgis, *Quantum dynamics of an excess proton in water using an extended empirical valence-bond Hamiltonian*, Journal of Physical Chemistry B **102**, 1998 (4261).

- [96] R. Vuilleumier and D. Borgis, *An extended valence bond model for describing proton transfer in  $H^+$  ( $H_2O$ ) $_n$  clusters and liquid water*, Chemical Physics Letters **284**, 1998 (71).
- [97] R. Vuilleumier and D. Borgis, *Molecular Dynamics of an excess proton in water using a non-additive valence bond force field*, Journal of Molecular Structure **436-437**, 1997 (555).
- [98] R. Vuilleumier, V. Ego, L. Neltner and A.-M. Cazabat, *Tears of Wine : The Stationary State*, Langmuir **11**, 1995 (4117).
- [99] W. J. Wild, E. J. Kibblewhite and R. Vuilleumier, *Sparse matrix wave-front estimators for adaptive-optics systems for large-ground-based telescopes*, Optics Letters **20**, 1995 (955).

## 2. Actes de congrès à comité de lecture

- [1] Sanctis, M. L. de, M.-F. Politis, R. Vuilleumier, C. R. Stia, et O. A. Fojón. *Model Potentials in Liquid Water Ionization by Fast Electron Impact*. J. of Phys. : Conf. Ser. 583 (1) : 012023 (2015) [doi:10.1088/1742-6596/583/1/012023](https://doi.org/10.1088/1742-6596/583/1/012023) .
- [2] Sanctis, M. L. de, Politis, M.-F., Vuilleumier, R., Stia, C. and Fojón, O. *Triple differential cross sections for liquid water ionization by impact of fast electrons*. J. Phys. : Conf. Ser. 488, 052024 (2014).
- [3] López-Tarifa, P., Piekarski, G. D., Rossich, E., Hervé du Penhoat, M.-A., Vuilleumier, R., Gageot, M.-P., Tavernelli, I., Politis, M.-F., Wang, Y., Diaz-Tendero, S., Martin, F. and Alcamí, M. *Ultrafast nonadiabatic fragmentation dynamics of biomolecules*. J. Phys. : Conf. Ser. 488, 012037 (2014).
- [4] O A Fojón, M L de Sanctis, R Vuilleumier, C R Stia and M -F Politis, *Ionization of liquid water by fast electron impact : multiple differential cross sections for the 1B1 orbital*. Journal of Physics : Conference Series 288, 012010 (2011).
- [5] M.E. Galassi, M.P. Gageot, B. Gervais, M. Beuve, R. Vuilleumier, P.D. Fainstein, C.R. Stia, M.F. Politis *Multiple Ionization Processes Related to Irradiation of Biological Tissue in Photonic, Electronic and Atomic Collisions – Proceedings of the XXIV Conference* (World Scientific Publishing Co. Pte. Ltd., Singapore, 2006), P.482
- [6] S. Pommeret, J.P. Renault, S. Le Caër, G. Vigneron, R. Vuilleumier, S. Bratos and J.-Cl. Leicknam *Role of the H bond network in the radiation chemistry of hydrated systems in Trombay Symposium on Radiation and PhotoChemistry* T. Mukeherjee ed. (2006), vol. 1 p. 11.
- [7] M. Kozinski, W. Jarzeba and R. Vuilleumier *Solvation dynamics of coumarin 153 in benzene-acetonitrile and benzene-methanol mixtures : a Molecular Dynamics study in Femtochemistry and Femtobiology*, M. Martin et J. T. Hynes eds. (Elsevier, 2004), p245.
- [8] M. Wulff, M. Lorenc, A. Plech, H. Ihee, S. Bratos, F. Mirloup and R. Vuilleumier *Time-resolved x-ray diffraction from small molecules in solution in Femtochemistry and Femtobiology*, M. Martin et J. T. Hynes eds. (Elsevier, 2004), p337.
- [9] F. Mirloup, R. Vuilleumier, S. Bratos, M. Wulff and A. Plech *Time-dependent x-ray scattering signal of laser heated liquids in Femtochemistry and Femtobiology*, M. Martin et J. T. Hynes eds. (Elsevier, 2004), p349.

## 3. Publications à large audience

- [1] D. Borgis, A. Boutin and R. Vuilleumier, *Une solution pour les liquides : la statistique moléculaire*, Actualité chimique 382-383, 71-77 (2014).

- [2] R. Vuilleumier and D. Borgis, *News and Views : Hopping along hydrogen bonds*, Nature Chemistry 4, 432 (2012).
- [3] A. Boutin and R. Vuilleumier *De Boltzmann aux expériences « in silico »*, Actualité chimique 353-54, 61-65 (2011).

#### 4. Chapitres de livre

- [1] J.-L. Barrat and R. Vuilleumier *A guide to statistical physics issues in molecular simulations*, dans *Neutrons et simulations (école thématique de la SFN)*, M. Johnson, N. Malikova et M. Plazanet éditeurs (EDP Sciences)
- [2] R. Vuilleumier *Density Functional Theory based ab initio Molecular Dynamics using the Car-Parrinello approach*, dans *Computer Simulations in Condensed Matter : From Materials to Chemical Biology (Lecture Notes in Physics)*, M. Ferrario, G. Ciccotti et K. Binder éditeurs (Springer, 2006), chapitre 8.
- [3] R. Vuilleumier and D. Borgis, *Modelling proton transfer in solution using non-additive valence bond force fields*, B. J. Berne, G. Ciccotti and D. F. Coker eds.(World Scientific Publishing Co. Ltd., London, 1998).