

PUBLICATIONS

Liste de publications dans des revues à comité de lecture

- 1999 1. N. Suaud, H. Bolvin, J.-P. Daudey, "Ab initio Calculations of the Magnetic Coupling between a Ni(II) Ion and Two Nitroxyde Radicals", **Inorg. Chem.**, 6089, 38 (1999).
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- 2001 3. M.-B. Lepetit, N. Suaud, "Ab initio evaluation of the local effective interactions in α' NaV₂O₅", **Int. J. Mod. Phys. B**, 1377, 15 (2001)
- 2002 4. N. Suaud, M.-B. Lepetit, "Ab initio evaluation of the charge ordering in α' NaV₂O₅", **Phys. Rev. Letters**, 056405, 88 (2002).
5. I. de P. R. Moreira, N. Suaud, N. Guihéry, J. P. Malrieu, R.. Caballol, J. M. Bofill, F. Illas, "Derivation of spin Hamiltonians from the exact Hamiltonian : Application to systems with two unpaired electrons per magnetic site", **Phys. Rev. B**, 134430, 66 (2002).
6. N. Suaud, A. Gaita-Ariño, J. M. Clemente-Juan, J. Marín-Sánchez, E. Coronado, "Electron delocalization in mixed-valence Keggin polyoxometalates. Ab initio calculation of the local effective transfer integrals and its consequences on the spin coupling.", **J. Am. Chem. Soc.**, 15134, 124 (2002).
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8. N. Suaud, A. Gaita-Ariño, J. M. Clemente-Juan, J. Marín-Sánchez, E. Coronado, "Ab initio calculations of the transfer parameters and coulombic repulsion and estimation of their effects on the electron delocalization and magnetic coupling in mixed-valence Keggin polyoxotungstates", **Polyhedron** 2331, 22 (2003).
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- 2004 10. N. Suaud, A. Gaita-Ariño, J. M. Clemente-Juan, E. Coronado, "Electron Delocalization and Electrostatic Repulsion at the Origin of the Strong Spin Coupling in Mixed-Valence Keggin Polyoxometalates. Ab initio Calculations of the One and Two Electron Processes", **Chem. Euro. J.**, 4041, 10 (2004).
11. S. Evangelisti, N. Guihéry, T. Leininger, J.-P. Malrieu, D. Maynau, J.-V. Pitarch-Ruiz, N. Suaud, C. Angeli, R. Cimiraglia, C. J. Calzado, "Local Orbitals for Quasi-Degenerated Systems", **J. Mol. Struc. : Theochem**, 1, 709 (2004).
- 2006 12. R. Bastardis, N. Guihéry, N. Suaud, C. de Graaf, "Competition between double exchange and purely magnetic Heisenberg models in mixed valence systems : Application to half-doped manganites", **J. Chem. Phys.**, 194708, 125 (2006).
- 2007 13. R. Bastardis, N. Guihéry, N. Suaud, "Relation between double exchange and Heisenberg model spectra : Application to the half-doped manganites", **Phys. Rev. B**, 132403, 75 (2007).
14. J.M. Clemente-Juan, E. Coronado, A. Gaita-Ariño, N. Suaud, "Mixed-Valence Polyoxometalates : Spin Coupling and Electron Distribution in the Decawolframate Anion Reduced by Two Electrons", **J. Phys. Chem. A**, 9969, 111 (2007).
- 2008 15. C. J. Calzado, J. M. Clemente-Juan, E. Coronado, A. Gaita-Ariño, N. Suaud, "Role of electron transfer and magnetic exchange interactions in the magnetic properties of mixed-valence polyoxovanadate complexes", **Inorg. Chem.**, 5889, 47 (2008).
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19. N. Suaud, Y. Masaro, E. Coronado, J. M. Clemente-Juan, N. Guihéry, "Origin of the paramagnetic properties of a two-electron reduced V_{14} polyoxometalate : wave function theory and model hamiltonian calculations." **Eur. J. Inorg. Chem.**, 5109, (2009).
20. R. Maurice, R. Bastardis, C. de Graaf, N. Suaud, T. Mallah, N. Guihéry, "Universal theoretical approach to extract anisotropic spin Hamiltonians", **J. Chem. Theo. Comput.**, 2977, 5 (2009).
- 2010 21. C. Boilleau, N. Suaud, R. Bastardis, N. Guihéry, J.P. Malrieu "Possible use of DFT approaches for the determination of double exchange interactions." **Theo. Chem. Accounts**, 231, 126 (2010).
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27. T. Krah, N. Suaud, A. Zanchet, V. Robert, N. Ben Amor, "Vacancy-induced electron transfer in FeCo Prussian blue analogue : a theoretical investigation", **Eur. J. Inorg. Chem.**, 5777, 35 (2012).
28. C. Boilleau, N. Suaud, N. Guihéry, "Ab initio study of the influence of structural parameters on the potential energy surfaces of spin-crossover Fe(II) model compounds", **J. Chem. Phys.**, 224304, 137 (2012).
- 2013 29. S. Cardona-Serra, J.M. Clemente-Juan, A. Gaita-Ariño, N. Suaud, O. Svoboda, E. Coronado, "Electric field control of the spin state in the mixed-valence polyoxometalate $[GeV_{14}O_{40}]^{8-}$ ", **Chem. Com.**, 9621, 49 (2013).
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« Very Important Paper »
32. N. Suaud, X. López, N. Ben Amor, N. Bandeira, C. de Graaf, J.M. Poblet « Accuracy of Embedded Fragment Calculation for evaluating Electron Interactions in Mixed Valence Magnetic Systems : Study of 2e-reduced Lindqvist Polyoxometalates », **J. Comput. Theo. Chem.**, 550, 11 (2015).
33. B. Pradines, N. Suaud, J.P. Malrieu, "In Search of a Rational Dressing of Intermediate Effective Hamiltonians", **J. Phys. Chem. A**, 5207, 119 (2015).
- 2016 34. L. Dontot, N. Suaud, M. Rapacioli, F. Spiegelman, « An extended DFTB-CI model for charge-transfer excited states in cationic molecular clusters : model studies against ab initio calculations in small PAH clusters », **Phys. Chem. Chem. Phys.**, 18, 3545 (2016).
35. V. Chilkuri, N. Suaud, N. Guihéry, « High-Spin Chains and Crowns from Double-exchange Mechanism », **Crystals**, 6, 39 (2016).
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 39. **N. Suaud**, J.P. Malrieu, « *Natural Molecular Orbitals : limits of a Lowdin's conjecture* », **Mol. Phys.** , 115, 2684-2695 (2017).
 40. L. Escalera-Moreno, N. Suaud, A. Gaita-Ariño, E. Coronado, "Determining Key Local Vibrations in the Relaxation of Molecular Spin Qubits and Single Molecule Magnets", **J. Phys. Chem. Letters**, 8, 1695-1700 (2017).
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 - 2018 43. B. Pradines, L. Lacombe, N. Guihéry, **N. Suaud**, "Study of the electronic Structure of $NiGa_2S_4$ and extraction of the spin Hamiltonian parameters from *ab initio* calculations", **Euro. J. Inorg. Chem.**, 2018, 503-508 (2018).
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 45. W. Salomon, E. Rivière, X. López, **N. Suaud**, P. Mialane, M. Haouas, A. Saad, J. Marrot, and A. Dolbecq, "Bicapped Keggin polyoxomolybdates : discrete species and experimental and theoretical investigations on the electronic delocalization in a chain compound", **Dalton Trans.** , publié en ligne.
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 47. L. Brooke, A. Diaz-Marquez, S. Evangelisti, Th. Leininger, P.-F. Loos, **N. Suaud**, and J. A. Berger, "Distributed gaussian orbitals for the description of electrons in an external potential", **J. Mol. Model.**, accepté.
- A soumettre 1. S. Forel, F. Bouanis, G. Magadur, S. Das, A. Baron, Ch. Herrero, A. Quaranta, G. Delport, B. Vauzeilles, V. Huc, M. Sircoglou, J.-S. Lauret, W. Leibl, M. Bouammali, **N. Suaud**, N. Guihéry, C.-S. Cojocaru, A. Aukauloo, T. Mallah "Visible light induced large, fast and reversible switch of the conductivity via cascade triplet-triplet energy transfer in SWNT-FET devices decorated with photoactive complexes", à soumettre à **Advanced Functional Materials**

Actes de congrès

1. A. Gaita-Ariño, S. Cardona-Serra, J. Clemente-Juan, E. Pinilla-Cienfuegos, **N. Suaud**, J. Palacios, "Magnetic polyoxometalates in molecular electronics", **International Chemical Congress of Pacific Basin Societies**, Dec 2010, Honolulu, HI, United States ;
2. E. Coronado, S. Cardona-Serra, J. Clemente-Juan, E. Pinilla-Cienfuegos, **N. Suaud**, "Polyoxometalates in molecular spintronics" **International Chemical Congress of Pacific Basin Societies**, Dec 2010, Honolulu, HI, United States.