

Emmanuel FROMAGER – Publications

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Publi. 51: “Unitary transformations within density matrix embedding approaches: A perspective on the self-consistent scheme for electronic structure calculation”– Q. Marécat, B. Lasorne, E. Fromager, and M. Saubanère *Phys. Rev. B* **108**, 155119 (2023), Preprint: [arxiv:2306.07641](https://arxiv.org/abs/2306.07641)

Publi. 50: “A unified density-matrix functional construction of quantum baths in density matrix embedding theory beyond the mean-field approximation”– S. Sekaran, O. Bindech, and E. Fromager, *J. Chem. Phys.* **159**, 034107 (2023), Preprint: [arXiv:2304.14729](https://arxiv.org/abs/2304.14729)

Publi. 49: “Quantum embedding of multi-orbital fragments using the Block-Householder-transformation”– S. Yalouz, S. Sekaran, E. Fromager, and M. Saubanère, *J. Chem. Phys.* **157**, 214112 (2022), Preprint: [arXiv:2209.10302](https://arxiv.org/abs/2209.10302)

Publi. 48: “DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science”– Andrew M. Teale, Trygve Helgaker, Andreas Savin, Carlo Adamo, Bálint Aradi, Alexei V. Arbuznikov, Paul W. Ayers, Evert Jan Baerends, Vincenzo Barone, Patrizia Calaminici, Eric Cancès, Emily A. Carter, Pratim Kumar Chattaraj, Henry Chermette, Ilaria Ciofini, T. Daniel Crawford, Frank De Proft, John F. Dobson, Claudia Draxl, Thomas Frauenheim, **Emmanuel Fromager**, Patricio Fuentealba, Laura Gagliardi, Giulia Galli, Jiali Gao, Paul Geerlings, Nikitas Gidopoulos, Peter M. W. Gill, Paola Gori-Giorgi, Andreas Görling, Tim Gould, Stefan Grimme, Oleg Gritsenko, Hans Jørgen Aagaard Jensen, Erin R. Johnson, Robert O. Jones, Martin Kaupp, Andreas M. Köster, Leeor Kronik, Anna I. Krylov, Simen Kvaal, Andre Laestadius, Mel Levy, Mathieu Lewin, Shubin Liu, Pierre-François Loos, Neepa T. Maitra, Frank Neese, John P. Perdew, Katarzyna Pernal, Pascal Pernot, Piotr Piecuch, Elisa Rebolini, Lucia Reining, Pina Romaniello, Adrienn Ruzsinszky, Dennis R. Salahub, Matthias Scheffler, Peter Schwerdtfeger, Viktor N. Staroverov, Jianwei Sun, Erik Tellgren, David J. Tozer, Samuel B. Trickey, Carsten A. Ullrich, Alberto Vela, Giovanni Vignale, Tomasz A. Wesolowski, Xin Xu, and Weitao Yang, *Phys. Chem. Chem. Phys.* (2022) **24**, 28700–28781, Advance Article, DOI: 10.1039/d2cp02827a [2022 HOT PCCP article: [link](https://doi.org/10.1039/d2cp02827a)], Preprint: [10.26434/chemrxiv-2022-13j2v](https://arxiv.org/abs/2022.13j2v)

Publi. 47: “Reduced density matrix functional theory from an ab initio seniority-zero wave function: Exact and approximate formulations along adiabatic connection paths”– B. Senjean, S. Yalouz, N. Nakatani, and E. Fromager, *Phys. Rev. A* **106**, 032203 (2022), Preprint: [arXiv:2204.00699](https://arxiv.org/abs/2204.00699)

Publi. 46: “Local Potential Functional Embedding Theory: A Self-Consistent Flavor of Density Functional Theory for Lattices without Density Functionals”– S. Sekaran, M. Saubanère, and E. Fromager, *Computation* **2022**, *10*, 45. [invited paper in the special issue of *Computation* in honour of Karlheinz Schwarz on the occasion of his 80th birthday] Preprint: [arXiv:2202.08071](https://arxiv.org/abs/2202.08071)

Publi. 45: “Ensemble Density Functional Theory of Neutral and Charged Excitations”– F. Cernatic, B. Senjean, V. Robert, and E. Fromager, *Top Curr Chem (Z)* **380**, 4 (2022), *review article in the “New Horizon in Computational Chemistry Software” topical collection*. Also published as a [book chapter](#), preprint: [arXiv:2109.04943](https://arxiv.org/abs/2109.04943)

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Publi. 43: “Exact exchange–correlation potentials for calculating the fundamental gap with a fixed number of electrons”– M. J. P. Hodgson, J. Wetherell, and E. Fromager, *Phys. Rev. A* **103**, 012806 (2021), Preprint: [arXiv:2010.05642](https://arxiv.org/abs/2010.05642)

Publi. 42: “New approaches to study excited states in density functional theory: general discussion”– Jan Gerit Brandenburg, Kieron Burke, Emmanuel Fromager, Matteo Gatti, Sara Giarrusso, Nikitas I Gidopoulos, Paola Gori-Giorgi, Duncan Gowland, Trygve Helgaker, Matthew JP

Hodgson, Lionel Lacombe, Gianluca Levi, Pierre-François Loos, Neepa T Maitra, Eduardo Maurina Morais, Nisha Mehta, Filippo Monti, Manasi R Mulay, Katarzyna Pernal, Lucia Reining, Pina Romaniello, Matthew R Ryder, Andreas Savin, Dumitru Sirbu, Andrew M Teale, Alex JW Thom, Donald G Truhlar, Jack Wetherell, Weitao Yang, *Faraday Discuss.*, 2020, **224**, 483–508.

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Publi. 38: “A weight-dependent local correlation density-functional approximation for ensembles” – P.-F. Loos and E. Fromager, *J. Chem. Phys.* **152**, 214101 (2020), **JCP Editor's Pick**, Preprint: [arXiv:2003.05553](https://arxiv.org/abs/2003.05553)

Publi. 37: “Individual Correlations in Ensemble Density Functional Theory: State- and Density-Driven Decompositions without Additional Kohn-Sham Systems” – E. Fromager, *Phys. Rev. Lett.* **124**, 243001 (2020), Preprint: [arXiv:2001.08605](https://arxiv.org/abs/2001.08605) [[Supplemental Material](#)]

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Publi. 35: “Site-occupation-Green's function embedding theory: A density-functional approach to dynamical impurity solvers” – L. Mazouin, M. Saubanière, and E. Fromager, *Phys. Rev. B* **100**, 195104 (2019).

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Publi. 33: “Multiple impurities and combined local density approximations in Site-Occupation Embedding Theory” – B. Senjean, N. Nakatani, M. Tsuchiizu, and E. Fromager, *Theor. Chem. Acc.* (2018) 137: 169 [**special issue in memoriam of Janos Angyan**].

Publi. 32: “Unified formulation of fundamental and optical gap problems in density-functional theory for ensembles” – B. Senjean and E. Fromager, *Phys. Rev. A* **98**, 022513 (2018).

Publi. 31: “Exploring weight-dependent density-functional approximations for ensembles in the Hubbard dimer” – K. Deur, L. Mazouin, B. Senjean, and E. Fromager, *Eur. Phys. J. B* **91**, 162 (2018) [**special issue in honour of Hardy Gross**].

Publi. 30: “Site-Occupation Embedding Theory using Bethe Ansatz Local Density Approximations” – B. Senjean, N. Nakatani, M. Tsuchiizu, and E. Fromager, *Phys. Rev. B* **97**, 235105 (2018).

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[Publi. 28](#): “Electron transport through a Spin Crossover junction. Perspectives from a wavefunction-based approach” – S. Vela, M. Vérot, E. Fromager, and V. Robert, *J. Chem. Phys.* **146**, 064112 (2017).

[Publi. 27](#): “Exact ensemble density functional theory for excited states in a model system: Investigating the weight dependence of the correlation energy” – K. Deur, L. Mazouin, and E. Fromager, *Phys. Rev. B* **95**, 035120 (2017).

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[Publi. 22](#): “On the exact formulation of multi-configuration density-functional theory: electron density versus orbitals occupation” – E. Fromager, *Mol. Phys.* **113**, 419 (2015) [**Invited 'New Views' paper**[Author profile](#)].

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[Publi. 14](#): “Metallophilic interactions in A-frame molecules [S(MPH₃)₂] (M = Cu, Ag, Au) from range-separated density-functional perturbation theory” – M. M. Alam and E. Fromager, *Chem. Phys. Lett.* **554**, 37 (2012).

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