**Emmanuel FROMAGER - Publications**

[ResearcherID: M-4727-2017](http://www.researcherid.com/rid/M-4727-2017) [Google Scholar](https://scholar.google.fr/citations?user=6S8Or18AAAAJ&hl=fr)

[Publi. 51:](https://doi.org/10.1103/PhysRevB.108.155119) “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:](https://doi.org/10.1063/5.0157746) “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:](https://doi.org/10.1063/5.0125683) “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:](https://doi.org/10.1039/D2CP02827A) “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://pubs.rsc.org/en/Journals/ArticleCollectionLanding?themeId=e3d7e371-bed8-4ccd-bd58-1d9ee83cec7e&journalName=)**]**, Preprint: [10.26434/chemrxiv-2022-13j2v](https://chemrxiv.org/engage/chemrxiv/article-details/62974da519595958f0bcc339)

[Publi. 47:](https://doi.org/10.1103/PhysRevA.106.032203) “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:](https://doi.org/10.3390/computation10030045) “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:](https://doi.org/10.1007/s41061-021-00359-1) “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](https://doi.org/10.1007/978-3-031-07658-9_8), preprint: [arXiv:2109.04943](https://arxiv.org/abs/2109.04943)

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[Publi. 37:](https://link.aps.org/doi/10.1103/PhysRevLett.124.243001) “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](https://quantique.u-strasbg.fr/lib/exe/fetch.php?media=fr:pageperso:ef:supp_mat_for_revision.pdf)]

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