

Emmanuel FROMAGER – Publications (updated September 2024)

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Publi. 55: “Fragment quantum embedding using the Householder transformation: A multi-state extension based on ensembles”– F. Cernatic, E. Fromager, and S. Yalouz, *J. Chem. Phys.* **161**, 124107 (2024). Preprint: [arXiv:2407.14278](https://arxiv.org/abs/2407.14278)

Publi. 54: “Neutral electronic excitations and derivative discontinuities: An extended N-centered ensemble density functional theory perspective”– F. Cernatic, P.-F. Loos, B. Senjean, and E. Fromager, *Phys. Rev. B* **109**, 235113 (2024). Preprint: [arXiv:2401.04685](https://arxiv.org/abs/2401.04685)

Publi. 53: “Density functional theory beyond the Born–Oppenheimer approximation: exact mapping onto an electronically non-interacting Kohn–Sham molecule”– E. Fromager and B. Lasorne, 2024 *Electron. Struct.* **6** 025002. Preprint: [arXiv:2312.15080](https://arxiv.org/abs/2312.15080)

Publi. 52: “Extended N-centered ensemble density functional theory of double electronic excitations”– F. Cernatic and E. Fromager, *J. Comput. Chem.* 2024;45:1945–1962. Preprint: [arXiv:2402.07161](https://arxiv.org/abs/2402.07161)

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, Leor 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](#)

Publi. 44: “Householder transformed density matrix functional embedding theory”– S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, *Phys. Rev. B* **104**, 035121 (2021), Preprint: [arXiv:2103.04194](#)

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](#)

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Publi. 41: “Weight Dependence of Local Exchange–Correlation Functionals in Ensemble Density-Functional Theory: Double Excitations in Two-Electron Systems”– C. Marut, B. Senjean, E. Fromager, and P.-F. Loos, *Faraday Discuss.*, 2020, **224**, 402–423, Preprint: [arXiv:2005.06159](#)

Publi. 40: “Strong correlation in density functional theory: general discussion”– Emmanuel Fromager, Nikitas Gidopoulos, Paola Gori-Giorgi, Trygve Helgaker, Pierre-François Loos, Thomas Malcomson, Katarzyna Pernal, Andreas Savin, Donald G Truhlar, Meilani Wibowo, Weitao Yang, *Faraday Discuss.*, 2020, **224**, 373–381.

Publi. 39: “New density–functional approximations and beyond: general discussion”– Jan Gerit Brandenburg, Kieron Burke, Antonio Cancio, Jannis Erhard, Emmanuel Fromager, Abhisek Ghosal, Nikitas Gidopoulos, Paola Gori-Giorgi, Trygve Helgaker, Ben Hourahine, Christoph R Jacob, Derk Kooi, Neepa Maitra, Manasi R Mulay, Katarzyna Pernal, Aurora Pribram-Jones, Lucia Reining, Pina Romaniello, Matthew R Ryder, Andreas Savin, Chris-Kriton Skylaris, Andrew M Teale, David Tozer, Donald G Truhlar, Weitao Yang, *Faraday Discuss.*, 2020, **224**, 166–200.

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](#)

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

Publi. 34: “Ground and excited energy levels can be extracted exactly from a single ensemble density–functional theory calculation” – K. Deur and E. Fromager, *J. Chem. Phys.* **150**, 094106 (2019).

[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).

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[Publi. 29](#): “Combining extrapolation with ghost interaction correction in range–separated ensemble density functional theory for excited states” – Md. M. Alam, K. Deur, S. Knecht and E. Fromager, *J. Chem. Phys.* **147**, 204105 (2017).

[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).

[Publi. 26](#): “Local density approximation in site–occupation embedding theory” – B. Senjean, M. Tsuchiizu, V. Robert, and E. Fromager, *Mol. Phys.* **115**, 48 (2017). [**Molecular Physics Longuet–Higgins Early Career Researcher Prize 2017**]

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[Publi. 19](#): “Alternative separation of exchange and correlation energies in multi–configuration range–separated density–functional theory” – A. Stoyanova, A. M. Teale, J. Toulouse, T. Helgaker, and E. Fromager, *J. Chem. Phys.* **139**, 134113 (2013).

[Publi. 18](#): “Assessment of charge–transfer excitations with time–dependent range–separated density functional theory based on long–range MP2 and multiconfigurational self–consistent field

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