Emmanuel FROMAGER – Publications (updated October 2024)

ResearcherID: M-4727-2017 Google Scholar

Publi. 56: "Ensemble density functional theory of ground and excited energy levels"– E. Fromager (2024). Preprint: arXiv:2409.17000

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

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

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

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

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

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

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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

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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

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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

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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.

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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]**.

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