

Emmanuel FROMAGER – University of Strasbourg

List of publications (updated December 2025)

Google Scholar: <https://scholar.google.fr/citations?user=6S8Or18AAAAJ&hl=fr>
ResearcherID: <https://www.webofscience.com/wos/author/record/M-4727-2017>

Publi. 58: “Local Potential Functional Embedding Theory of Molecular Systems: Localized Orbital-Based Embedding from an Exact Density-Functional Perspective”– W. Makhlof, B. Senjean, and E. Fromager, *J. Chem. Theory Comput.* 2025, 21, 20, 10293–10314, Preprint: [arXiv:2507.19591](https://arxiv.org/abs/2507.19591)

Publi. 57: “Exact static linear response of excited states from ensemble density functional theory”– L. Dupuy and E. Fromager, *J. Phys. Chem. A* 2025, 129, 39, 9095–9109. Preprint: [arXiv:2506.16363](https://arxiv.org/abs/2506.16363)

Publi. 56: “Ensemble density functional theory of ground and excited energy levels”– E. Fromager, *J. Phys. Chem. A* 2025, 129, 4, 1143–1155. Preprint: [arXiv:2409.17000](https://arxiv.org/abs/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](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)

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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. Saubanière, *J. Chem. Phys.* **157**, 214112 (2022), Preprint: [arXiv:2209.10302](https://arxiv.org/abs/2209.10302)

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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. 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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