Emmanuel FROMAGER – University of Strasbourg

List of publications (updated September 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. Makhlouf, B. Senjean, and E. Fromager, *submitted to J. Chem. Theory Comput.* (under revision), Preprint: arXiv: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, in press. Preprint: arXiv: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

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

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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

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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

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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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