



Contribution ID: 15

Type: **not specified**

Response of materials to external perturbations under extreme conditions

Thursday 26 June 2025 11:30 (30 minutes)

The exchange-correlation (XC) functional is essential in Kohn-Sham density functional theory (KSDFT), while the kinetic energy functional is key in orbital-free DFT. We analyze these functionals by observing how materials respond to external perturbations [1-6]. Our new method computes the static XC kernel across any level of Jacob's ladder without functional derivatives, allowing us to explore XC kernels from local density approximations to hybrid functionals. This has led to the identification of parameters of hybrid functionals under high-pressure conditions. Currently, we are applying this approach to XC kernels in linear response time-dependent DFT to study the X-ray Thomson scattering spectrum of materials, collaborating closely with experimental teams [7-9]. This contribution highlights our methodological advancements and their applications under various conditions, from ambient to extreme, using high-power lasers.

- [1]Z. Moldabekov, M. Böhme, J. Vorberger, D. Blaschke, T. Dornheim, J. Chem. Theory Comput., 19, 1286-1299 (2023)
- [2]Z. Moldabekov, M. Lokamani, J. Vorberger, A. Cangi, T. Dornheim, J. Phys. Chem. Lett., 14, 1326-1333 (2023)
- [3]Z. Moldabekov, M. Lokamani, J. Vorberger, A. Cangi, T. Dornheim, The Journal of Chemical Physics, 158, (2023)
- [4]Z. Moldabekov, J. Vorberger, T. Dornheim, Progress in Particle and Nuclear Physics, 140, 104144 (2025)
- [5]Z. Moldabekov, J. Vorberger, T. Dornheim, J. Chem. Theory Comput., 18, 2900-2912 (2022)
- [6]Z. Moldabekov, S. Schwalbe, M. Böhme, J. Vorberger, X. Shao, M. Pavanello, F. Graziani, T. Dornheim, J. Chem. Theory Comput., 20, 68-78 (2023)
- [7]Z. Moldabekov, T. Gawne, S. Schwalbe, T. Preston, J. Vorberger, T. Dornheim, Phys. Rev. Research, 6, 023219 (2024)
- [8]Z. Moldabekov, T. Gawne, S. Schwalbe, T. Preston, J. Vorberger, T. Dornheim, ACS Omega, 9, 25239-25250 (2024)
- [9]T. Gawne, Z. Moldabekov, O. Humphries, K. Appel, C. Baetz, V. Bouffetier, E. Brambrink, A. Cangi, S. Göde, Z. Konôpková, M. Makita, M. Mishchenko, M. Nakatsutsumi, K. Ramakrishna, L. Randolph, S. Schwalbe, J. Vorberger, L. Wollenweber, U. Zastrau, T. Dornheim, T. Preston, Phys. Rev. B, 109, L241112 (2024)

Primary author: Dr MOLDABEKOV, Zhandos (Center for Advanced Systems Understanding | Helmholtz-Zentrum Dresden-Rossendorf)

Presenter: Dr MOLDABEKOV, Zhandos (Center for Advanced Systems Understanding | Helmholtz-Zentrum Dresden-Rossendorf)