Code Developments

Mariana Rossi

- Added functionality to restart mixer as many times as the user wants in a run.
- This seen to be advantageous on test systems, especially involving lanthanides and "cousins" MR !1956

Andrei Sobolev

- **BREAKING CHANGE:** Add internal implementation of PBEsol functional to the atomic solver; selected by default if user specifies xc pbesol MR!1958
- Fixes a discrepancy between libxc and FHI-aims, see issue 756 for more details, but introduces energy and derivative differences
- Can be reverted to the previous behaviour by setting atomic_solver_xc pbe

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Min-Ye Zhang

- Added support for exporting the dataset with perturbative SOC for LibRPA MR !1959
- Added documentation for ri_multipole_threshold keyword and improved the error message with a helpful hint when multiple non-zero multipoles are present in L-channel MR !1957
- Various bugfixes MR !1954 MR !1960

Jannis Kockläuner

- **New Feature**: Fully analytical version of the G_0W_0 self-energy for molecules
- Implements the fully analytical version of the G_0W_0 self-energy for closed-shell molecules at N^6 cost in the gw_exact module. It allows to compute quasiparticle energies and to print out self energies MR !1961

Francisco Delesma

- Added GPU support and real-space grid generation to separable RI MR !1963

- Enabled GPU support for separable RI operations using the COSMA library.
- Replaced the ScaLAPACK pseudo inversion with the ELSI–ELPA library, enabling GPU support.
- Added support for automated construction of radial shells via cubic splines, logspace sampling and Delley. This facilitates the automatic setup of real-space grids required for the separable RI approach.

Alberto Otero de la Roza

- Implemented fixed_volume option to relax_unit_cell for constant-volume relaxations MR !1966. When used, the trace of the stress tensor is subtracted, and the cell volume is fixed to prevent roundoff errors.

And other contributors, to whom we are grateful.

New Papers involving FHI-aims

Disclaimer: We compile this list by identifying recent publications that cite the 2009 FHI-aims paper (DOI: 10.1016/j.cpc.2009.06.022). Before including any publication, we verify that FHI-aims was used in some capacity within the article. If we have overlooked any published work involving FHI-aims, we apologize for the oversight and welcome you to inform us. This list is intended for informational purposes only.

- "Anisotropic Interlayer Potentials in C_3N/Graphene and C_3N/h-BN Heterostructures," H. Yang, B. Hu, W. Jiang, B. Wu, and W. Ouyang, J. Phys. Chem. C **129**(40), 18250–18260 (2025), DOI: 10.1021/acs.jpcc.5c04138.

- "High-Pressure Mg_3Cl_7 Synthesized in a Diamond Anvil Cell as a Polar Metal with Second-Harmonic Generation," Y. Yin, L. Dubrovinsky, F. Tasnádi, I.A. Abrikosov, A. Aslandukov, A. Aslandukova, F.I. Akbar, W. Zhou, F. Knoop, D. Laniel, A. Pakhomova, T. Fedotenko, K. Glazyrin, G. Garbarino, H. Fang, and N. Dubrovinskaia, J. Am. Chem. Soc. **147**(36), 32591–32599 (2025), DOI: 10.1021/jacs.5c07812.

- "High-temperature polymer composite capacitors with high energy density designed via machine learning," M. Yang, C. Wan, L. Zhou, X. Li, J. Pan, H. Li, J. Wang, W. Ren, B. Sun, E. Xu, Y. Xiao, M. Guo, M. Zhang, X. Li, J. Jiang, P. Hu, L. Duan, C.-W. Nan, Z. Shen, X. Wang, and Y. Shen, Nat Energy **10**(11), 1323–1333 (2025), DOI: 10.1038/s41560-025-01863-0.

- "Relating Structural and Optical Properties of Organic Thin Films on Chemically Inert Substrates," N. Kainbacher, P. Puschnig, and O.T. Hofmann, ACS Omega **10**(39), 45103–45112 (2025), DOI: 10.1021/acsomega.5c03920.

- "Stacking in Layered Covalent Organic Frameworks: A Computational Approach and PXRD Reference Guide," R. Steentjes, and E. Zojer, International Journal of Molecular Sciences **26**(18), 9222 (2025), DOI: 10.3390/ijms26189222.

- "The energy landscape of folding in n-$C_{14}H_{30}$ described by a machine-learned potential," T.C. Allison, J.M. Bowman, P.L. Houston, Y. Pillai, C. Qu, and D.J. Wales, J. Chem. Phys. **163**(10), 104307 (2025), DOI: 10.1063/5.0289549.

- "Theoretical Prediction of 2D Y_2CTI (T = Br, Cl, F, H) Janus MXene Monolayers for Photovoltaic Applications," B.D. Aparicio-Huacarpuma, C.M. de Oliveira Bastos, J.A.S. Laranjeira, F.L.L. Mendonça, A.M.A. Silva, J. R. Sambrano, A. Cavalheiro Dias, and L.A. Ribeiro Júnior, ACS Omega **10**(39), 45621–45632 (2025), DOI: 10.1021/acsomega.5c05916.

- "When Aromaticity Falls Short in Molecule–Surface Interactions," J. Brandhoff, R.K. Berger, F. Otto, M. Schaal, L. Brill, O.T. Hofmann, P. Puschnig, T. Fritz, and R. Forker, J. Phys. Chem. C **129**(46), 20738–20745 (2025), DOI: 10.1021/acs.jpcc.5c05441.

Upcoming Events

- Next FHI-aims monthly meeting: WEDNESDAY Nov 12, 2025 at 8:30 AM to 10:00 AM, Eastern Time, US and Canada, more details in the community Slack channel