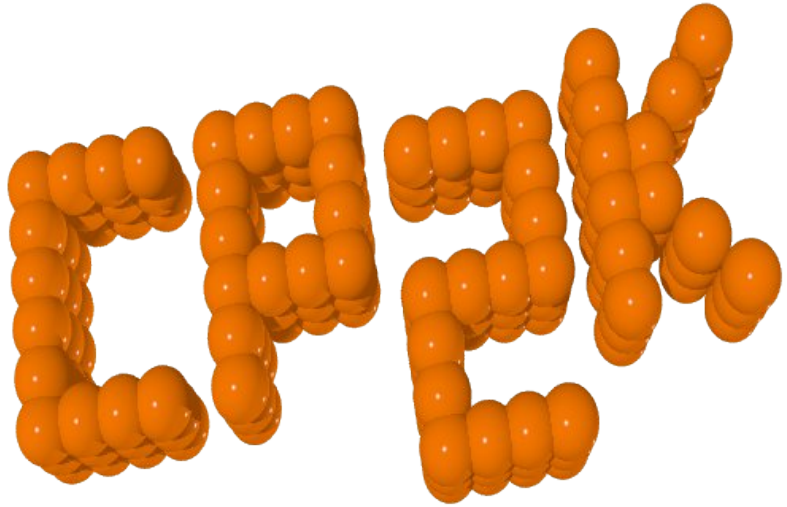
CP2K Developers Meeting

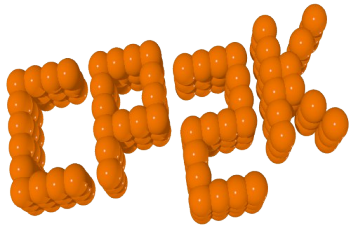
April 20th, 2026



Topics

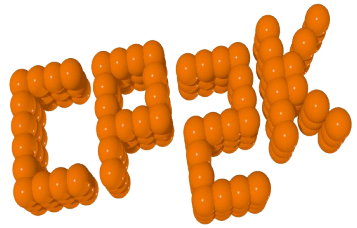
CP2K Developers Meeting

- New and Ongoing Developments
- Current Issues with CP2K
- Next CP2K Release
- Planned Events in the Context of CP2K



New and Ongoing Developments in CP2K

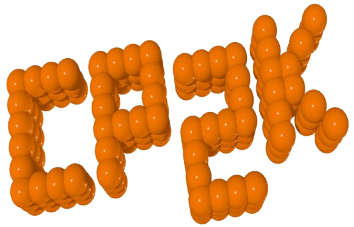
- LIB/XS/TREAM, and Low-Precision Compute (Hans Pabst)
- CP2K@CASUS
- RIXS (Beliz Sertcan)
- Efficient GW Computation Using Resolution of Identity Real-Space (RI-RS, Ritaj Tyagi)
- CP2K review spectroscopy and dynamics (Jan Wilhelm)
- CP2K HPC/benchmark paper (Frederick Stein, Robert Schade)
- Updates from Kiel / SPECAT group (Anna Hehn)



LIBXS, LIBXSTREAM, and Low-Precision Compute (1/3)

- Ported LIBXSMM usage in CP2K to LIBXS
  - LIBXSMM focuses on low-level code-generation only.
  - LIBXSMM/upstream removed API used in CP2K.
- LIBXS provides revised API for CP2K
  - Comprehensive, low-level, complete incl. Fortran interface.
  - Can leverage XSMM (X86, ARM, RISC-V) and MKL-JIT.

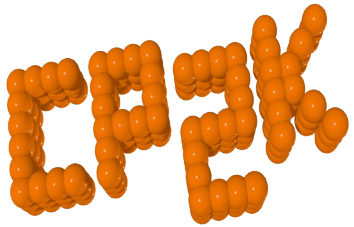
LIBXS: https://libxs.readthedocs.io/



LIBXS, **LIBXSTREAM**, and Low-Precision Compute (2/3)

- Optional GPU backend for DBCSR and CP2K
  - Previously: DBCSR provided OpenCL backend (*hackish*).
  - Implements CP2K offload and DBCSR ACC.
  - Open Source Low-Precision Compute.
- Sketch kernels for Low-Precision Compute, etc.
  - Presentation: https://libxs.readthedocs.io/ozaki/

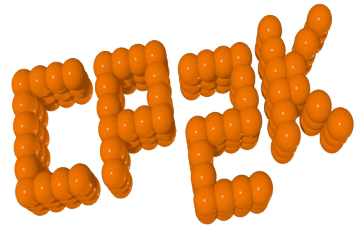
LIBXSTREAM: https://libxstream.readthedocs.io/



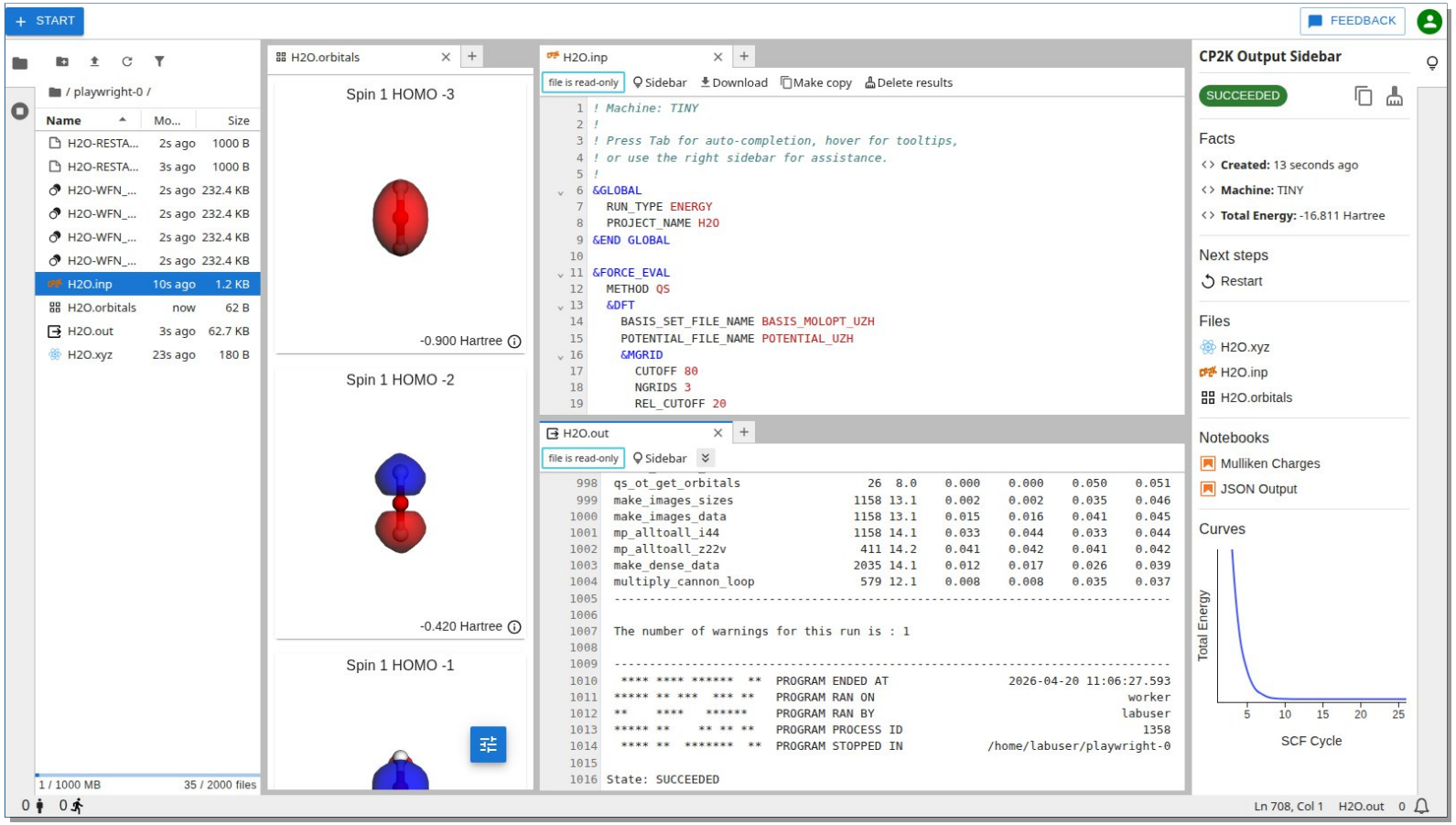
LIBXS, LIBXSTREAM, and **Low-Precision Compute** (3/3)

- Open Source Low-Precision (LP) Compute
  - **Presentation**: https://libxs.readthedocs.io/ozaki/
  - Statistical error analysis, e.g., CP2K workload.
  - Leverages LIBXSTREAM for GPU targets.
- Performance: supports CPU (AVX512-VNNI) and GPUs
  - Initial focus on statistical analysis

- Questions of interest
  - Can or should (effort) GPU kernels be written for LP?
  - Can GPUs hold the DP-crown going forward?



CP2K Lab

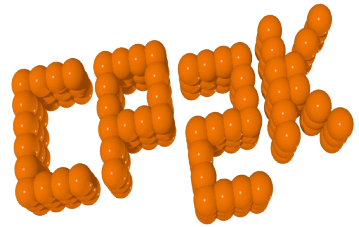


- Commercial GUI for CP2K
- Usability is CP2K's weak spot
- Usability is not publishable
- Committed to open science
- Try it (there's a free tier)

https://lab.cp2k.com

CP2K@CASUS (I)

- New FFT backend (WIP)
  - Better exploitation of libraries
  - Better starting point for GPU acceleration
  - Integration into CP2K yet missing
- cuSOLVERMp
- Active Space module
  - Better choice of selection methods
  - Restricted open-shell reference
- HPC Community Paper in progress -> see Robert Schade
- New Grassmann Extrapolation (see next slides)



Grassmann extrapolation

The mapping of interest: $\mathcal{F} : \mathcal{D} \longrightarrow \mathcal{T}_{\mathsf{D}_0}\mathcal{M}_{\mathrm{gr}}$, $d_{\mathbf{r}} \longmapsto \Gamma_{\mathbf{r}}$

Ansatz: For previous descriptors $d_{n-q}, \ldots, d_n$ and corresponding $\Gamma_i = \mathrm{Log}_{\mathrm{gr}}(\mathsf{D}_i)$, and the known descriptor d_{n+1} we search for approximations of the form

$$\Gamma_{n+1} \approx \tilde{\Gamma}_{n+1} := \sum_{i=0}^{q} \alpha_i \, \Gamma_{n-i},$$

with $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_n)$ solution to

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{q+1}} \left\| d_{n+1} - \sum_{i=0}^{q} \alpha_i d_i \right\|^2 + \varepsilon^2 \left\| \boldsymbol{\alpha} \right\|^2.$$

$$d_{n+1} \approx \sum_{i=0}^{q} \alpha_i \, d_{n-i}$$

$$\Downarrow$$

$$\Gamma_{n+1} \approx \sum_{i=0}^{q} \alpha_i \, \Gamma_{n-i}$$

$$\Downarrow$$

$$\mathsf{D}_{n+1} \approx \mathrm{Exp}_{\mathrm{gr}} \left(\sum_{i=0}^{q} \alpha_i \, \Gamma_{n-i} \right)$$

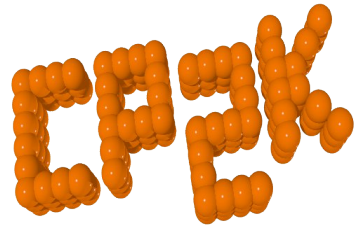
Then, the approximate $\mathsf{D}_{n+1} \approx \tilde{\mathsf{D}}_{n+1} = \mathrm{Exp}_{\mathrm{gr}}(\tilde{\Gamma}_{n+1}) \in \mathcal{M}_{\mathrm{gr}}$.

Does this work?

Rational: If the mapping $\mathcal{F} : \mathcal{D} \longrightarrow \mathcal{T}_{\mathsf{D}_0}\mathcal{M}_{\mathrm{gr}}$ was linear, then

$$\Gamma_{n+1} = \mathcal{F}(d_{n+1}) \approx \mathcal{F}\left(\sum_{i=0}^{q} \alpha_i d_i \right) = \sum_{i=0}^{q} \alpha_i \mathcal{F}\left(d_i\right) = \sum_{i=0}^{q} \alpha_i \Gamma_i.$$

More on this later...



Fixing the long-term drift by time-reversibility

Instead of exploiting the linearity

$$d_{n+1} \approx \sum_{i=0}^{q} \alpha_i \, d_{n-i} \qquad \Rightarrow \qquad \tilde{\Gamma}_{n+1} = \sum_{i=0}^{q} \alpha_i \, \Gamma_{n-i}$$

we now use the Ansatz

$$d_{n+1} + d_{n-q} \approx \sum_{i=0}^{\tilde{q}} \alpha_i \, (d_{n-i} + d_{n-q+i+1}) \qquad \Rightarrow \qquad \tilde{\Gamma}_{n+1} + \tilde{\Gamma}_{n-q} = \sum_{i=0}^{\tilde{q}} \alpha_i \, (\Gamma_{n-i} + \Gamma_{n-q+i+1})$$

Then, the approximate $\mathrm{D}_{n+1} \approx \tilde{\mathrm{D}}_{n+1} = \mathrm{Exp}_{\mathrm{gr}}(\tilde{\Gamma}_{n+1}) \in \mathcal{M}_{\mathrm{gr}}$.

A symmetric approximation provides a time-reversible initial guess.

Time-Reversible (TR G-Ext) initial guess:

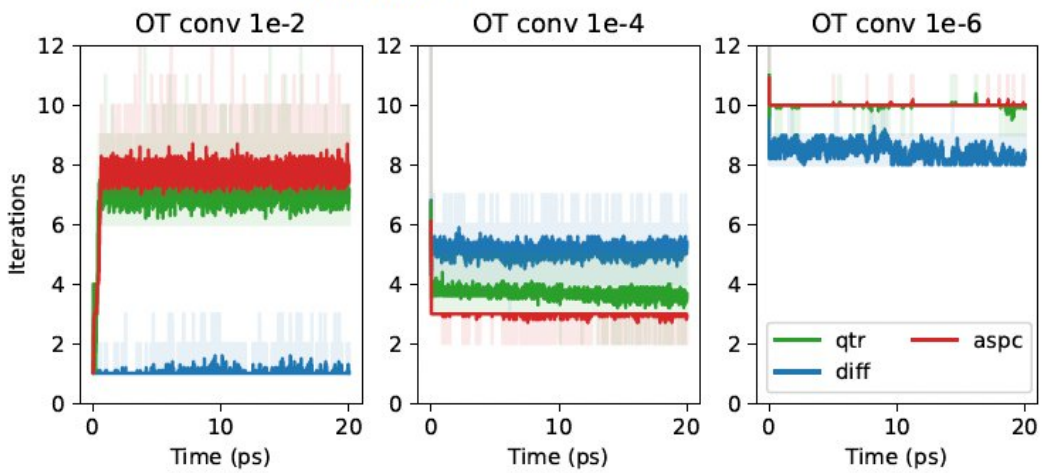
$$\tilde{\Gamma}_{n+1} := -\tilde{\Gamma}_{n-q} + \sum_{i=1}^{\tilde{q}} \alpha_i \, (\Gamma_{n-i} + \Gamma_{n-q+i})$$

Quasi Time-Reversible (QTR G-Ext) initial guess:

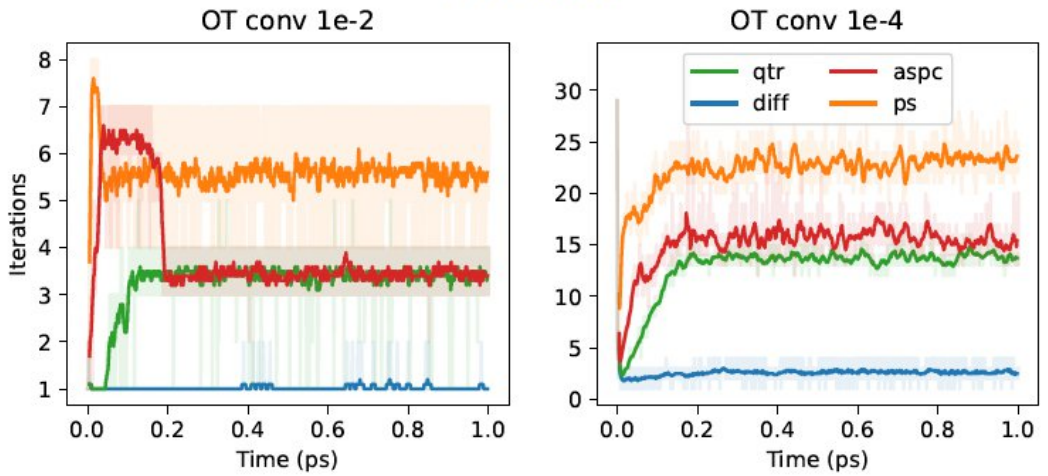
$$\tilde{\Gamma}_{n+1} := -\Gamma_{n-q} + \sum_{i=1}^{\tilde{q}} \alpha_i \, (\Gamma_{n-i} + \Gamma_{n-q+i})$$

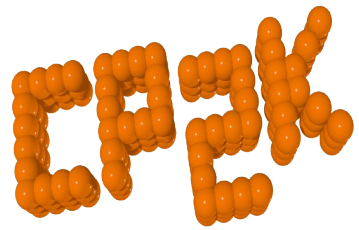
Strategy	OT convergence	Water		Silicon	
		Iter.	STD	Iter.	STD
ASPC+DIFF@DS	10^{-2}	1.02	0.16	1.02	0.13
ASPC+QTR@DS	10^{-2}	6.93	0.81	3.24	0.87
aspc	10^{-2}	7.61	0.94	3.85	1.15
ps	10^{-2}	—	—	5.58	1.12
ASPC+DIFF@DS	10^{-4}	5.14	0.64	2.59	1.20
ASPC+QTR@DS	10^{-4}	3.67	0.56	12.81	2.72
aspc	10^{-4}	2.98	0.25	15.14	2.65
ps	10^{-4}	—	—	22.32	2.52
ASPC+DIFF@DS	10^{-6}	8.42	0.50	—	—
ASPC+QTR@DS	10^{-6}	10.00	0.09	—	—
aspc	10^{-6}	10.00	0.05	—	—
ps	10^{-6}	—	—	65.05	16.79

Water:



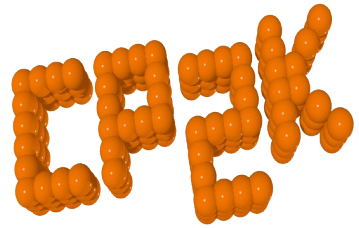
Silicon:





CP2K@CASUS (II)

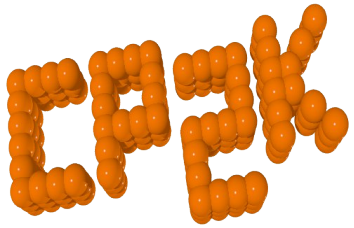
- Integration of TBlite
  - GFN2-xTB for periodic boundary conditions
- DFT-D4: parallelization?, debugging
- OpenPMD
- GauXC/Skala (see next slide)
- SPGLib-integration
- CP2K was awarded the Helmholtz Software Award (5,000 €)
- Kick-back to the CP2K community via CP2K Foundation: CP2K Award & Merch (via CASUS)
- Planned: EuroHPC Hackathon in Lugano (September)
  - Ideas? New FFT backend (WIP) or Full matrix operations
  - What are performance bottlenecks?
  - Ole: LibXC, GEEP



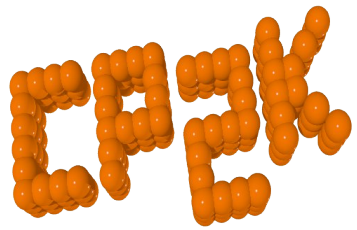
(WIP) Skala functional via GauXC, Franz Pöschel (CASUS)

- Skala:
  - deep-learning model for XC functionals
  - https://microsoft.github.io/skala
- GauXC:
  - library for evaluating XC/exact-exchange energy
  - Skala functional currently being integrated (currently still on a separate branch, named skala)
  - https://github.com/wavefunction91/gauxc
- Integrating GauXC into CP2K
  - https://github.com/cp2k/cp2k/pull/5084
  - Status: Full evaluation pipeline implemented, simulation converges, but results probably not yet correct (results are off roughly by a factor 2)
  - MPI awareness missing still
  - GauXC is more high-level than existing functionals (builds its own grid), so the code path is different compared to others

RIXS (Beliz Sertcan)



Efficient GW Computation Using Resolution of Identity Real-Space (RI-RS, Ritaj Tyagi)



Efficient GW Computation Using Resolution of Identity Real-Space (RI-RS)

RI-Vtr

$$(\mu\nu|P) = \int d\mathbf{r}\, \phi_\mu(\mathbf{r})\, \phi_\nu(\mathbf{r})\, v_P(\mathbf{r})\,,$$

$$v_P(\mathbf{r}) = \int d\mathbf{r}'\, v_{r_c}(\mathbf{r},\mathbf{r}')\, \varphi_P(\mathbf{r}')\,.$$

$$v_{r_c}(\mathbf{r},\mathbf{r}') = \begin{cases} 1/|\mathbf{r}-\mathbf{r}'| & \text{if } |\mathbf{r}-\mathbf{r}'| \le r_c\,, \\ 0 & \text{else}\,, \end{cases}$$

RI-RS

$$(\mu\nu|P)^{\text{RI-RS}} = \sum_{\mathbf{r}_\ell \in B^{\text{P}}} w_\ell\, \phi_\mu(\mathbf{r}_\ell)\, \phi_\nu(\mathbf{r}_\ell)\, v_P(\mathbf{r}_\ell)$$

$$= \sum_{\mathbf{r}_\ell \in B^{\text{P}}} \phi_\mu(\mathbf{r}_\ell)\, \phi_\nu(\mathbf{r}_\ell)\, Z_{\ell P}\,,$$

$$Z_{\ell P} = \underset{Z_{\ell P}}{\text{argmin}} \sum_{\mu\nu} \left[(\mu\nu|P) - (\mu\nu|P)^{\text{RI-RS}} \right]^2$$

$$\sum_{\ell'} D_{\ell\ell'}(\text{atom P})\, Z_{\ell' P} = d_{\ell P}$$

$$d_{\ell P} = \sum_{\mu\nu} \phi_\mu(\mathbf{r}_\ell)\, \phi_\nu(\mathbf{r}_\ell)\, (\mu\nu|P)$$

Linear system of equation : Parallelizable over atom P !!

Matrices are sparse : Use of efficient DBCSR operations

Computation of d_{lP} is $O(N)$ for large systems

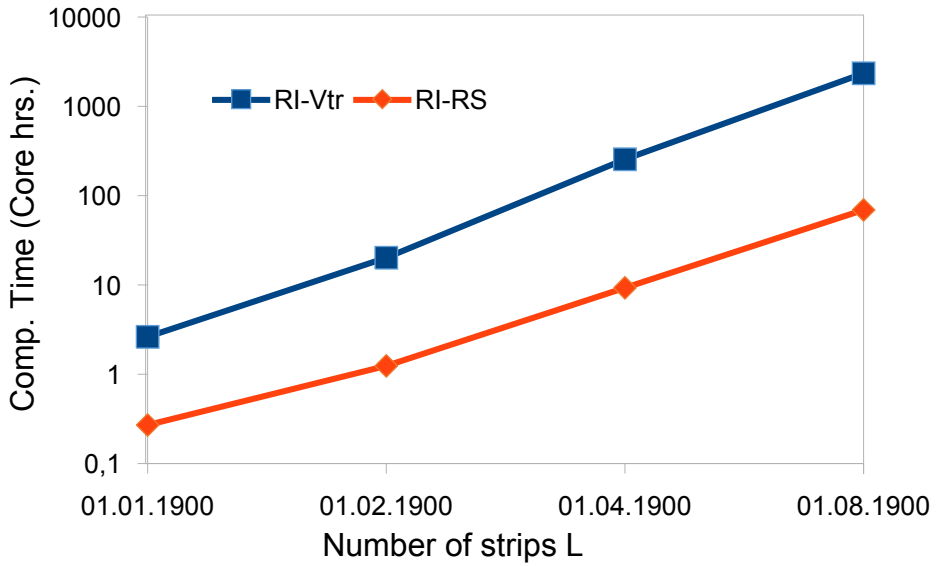
Wilhelm, J. *et al. J. Chem. Theory Comput.*, **2021**, 17, 3, 1662
Duchemin, I. *et al. J. Chem. Phys.*, **2019**, 150, 174120

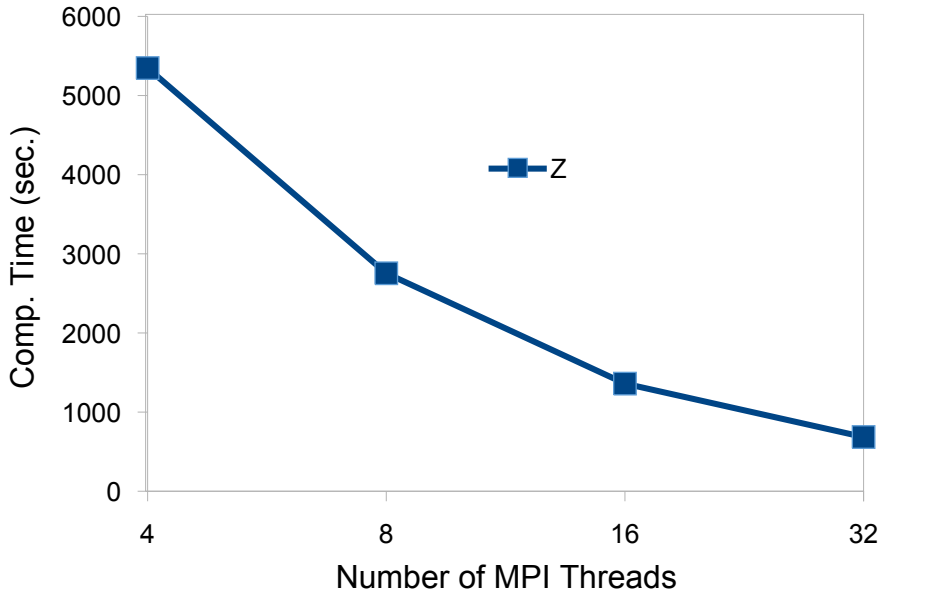
GW RI-RS : Results

Dataset	MAX (| RI-RS – RI-Vtr |)	
	IP	EA
GW100	2 meV	1 meV
ACC24	1 meV	1 meV
Nanographene	2 meV	1 meV

Matrices	Time (s)	
	RI-Vtr	RI-RS
Z	-	1360
$\chi(\imath\tau)$	1369	11
W	188	183
$\Sigma^{C}(\imath\tau)$	2870	10
Σ^{X}	1984	13

~3000 basis function ; 16 MPI / 8 OMP





GW RI-RS : Ongoing Work

- Implemented for molecules
  - - Periodic implementation ongoing (Full *k*-point sampling)
- Integration with RT-BSE for computation of spectroscopic properties of materials
- Grid points are available for all electron def2-TZVPP basis-set
  - - Seems to work well for basis set such as aug-cc-pVDZ, GTH basis set with
  - pseudopotential and basis set of less or similar quality as of def2-TZVPP
- Efficient grid generation ongoing
- This framework can used to accelerate HF, Hybrid, MP2 and RPA calculations anything
- that utilize 3-center RI integral framework

CP2K review spectroscopy and dynamics (JW)

RESEARCH ARTICLE | MAY 19 2020

CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations Editor's Pick

Special Collection: JCP Editors' Choice 2020 , Electronic Structure Software , Chemical Physics Software Collection

Thomas D. Kühne; Marcella Iannuzzi; Mauro Del Ben; Vladimir V. Rybkin; Patrick Seewald; Frederick Stein; Teodoro Laino; Rustam Z. Khaliullin; Ole Schütt; Florian Schiffmann; Dorothea Golze; Jan Wilhelm; Sergey Chulkov; Mohammad Hossein Bani-Hashemian; Valéry We Urban Borštnik; Mathieu Taillefumier; Alice Shoshana Jakobovits; Alfio Lazzaro; Hans Pabst; Tiziano Müller; Robert Schade; Manuel Guidon; Samuel Andermatt; Nico Holmberg; Gregory K. Schenter; Anna Hehn; Augustin Bussy; Fabian Belleflamme; Gloria Tabacchi; Andreas Glöß; Michael Lass; Iain Bethune; Christopher J. Mundy; Christian Plessl; Matt Watkins; Joost VandeVondele; Matthias Krack; Jürg Hutter

Check for updates

+ Author & Article Information

J. Chem. Phys. 152, 194103 (2020)

AIP Publishing **The Journal of Chemical Physics**

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Electronic Structure Software

Thanks to decades of developments and countless theoretical, methodological and algorithmic advances, many of them published in The Journal of Chemical Physics, the electronic structure community now has a wonderfully diverse arsenal of software packages available for performing calculations on molecules and materials. The calculations that can be performed with these packages range from high level predictions of the ground and excited electronic states of gas phase molecules, to "ab initio molecular dynamics" simulations of condensed phase materials, to the calculation of spectroscopic properties and experimental observables. Results from these codes have transformed our understanding of molecules and materials, have helped to guide the development of new materials, and to interpret and understand countless experimental results. The purpose of this Special Topic is to provide a single volume overview of some of the available electronic structure packages, of their functionalities, and of what makes each package unique.

Guest Editors: Angelos Michaelides, David Manolopoulos, Todd Martinez and David Sherrill

Codes in JCP „Electronic Structure Software“ Special Topic:

ORCA, PySCF, Molcas, TeraChem, CFOUR, CRYSTAL, SIESTA, DIRAC, TURBOMOLE, PSI4, ABINIT, DFTB+, Octopus, Molpro, GAMESS, Quantum Espresso, ONETEP, NWChem, WIEN2k

Recent JCP Software 2.0 Special Topic

Electronic Structure Software 2.0

Submission Deadline: June 30, 2026

Thanks to decades of effort by the electronic structure community, and numerous theoretical and algorithmic advances, many of them published in The Journal of Chemical Physics, researchers now have access…

MORE INFORMATION | CONTRIBUTE TO THIS SPECIAL TOPIC

CP2K: An electronic structure and molecular dynamics software package – Dynamics and Spectroscopy

Complementary to previous reviews:

RESEARCH ARTICLE | MAY 19 2020

CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations Editor's Pick

The Journal of Physical Chemistry B > Vol 130/Issue 4 > Article

Open Access | Editors' Choice

B: LIQUIDS; CHEMICAL AND DYNAMICAL PROCESSES IN SOLUTION | Jan

The CP2K Program Package Made Simple

CP2K HPC Benchmark Paper (Frederick Stein, Robert Schade)

Libraries/Functionality included:

– cusolvermp

– DLAF

– linear-scaling solver (incl. DBCSR, OpenPMD)

– SIRIUS

– HF & EXX

– RPA

– GW

Jour-Fixe every second Friday (next 24.4 14-15:00, https://uni-paderborn-de.zoom-x.de/j/68024819995?pwd=K6bDTJnBqES9edVxD6fpQ4bV0T9akq.1)

Updates from Kiel / SPECAT group

Finished / to be submitted:

- Fragmented intrinsic atomic orbitals / ROSE interface (Lukas Guhl, F3 lab student)
- Different smearing functions (Marisa Schneider, Master student; Collaboration with Prof. Wächtler)
- Transition dipole moments for the NewtonX-CP2K interface (Dr. Luis Cardenas, visiting researcher)

Still to be improved and published features:

- Smeared occupation TDA gradients
- sBSE and Bethe-Salpeter kernels gradients
- CP2K-Newton-X-WaveMixings interface
- Full TDDFT / ATDA (PhD student Tejas Thorat)

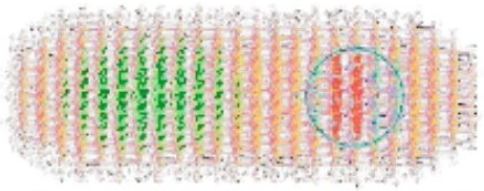
Additional developments to be pursued:

- QM/MM for TDDFT module (EnvironEX^2) and developments for GFN-xTB

Updates from Kiel / SPECAT group

EnvironEX² - Treating ENVIRONments when modelling EXcited states in EXtended systems

Modelling 1. CdSe@CdS nanorods



20-70 nm size range

Reassessing with improved GFN2-xTB semi-empirics

CP2K

xTB
$\mathbf{FC} = \mathbf{SC}\varepsilon$

sTDA
$\mathbf{AX} = \omega\mathbf{X}$

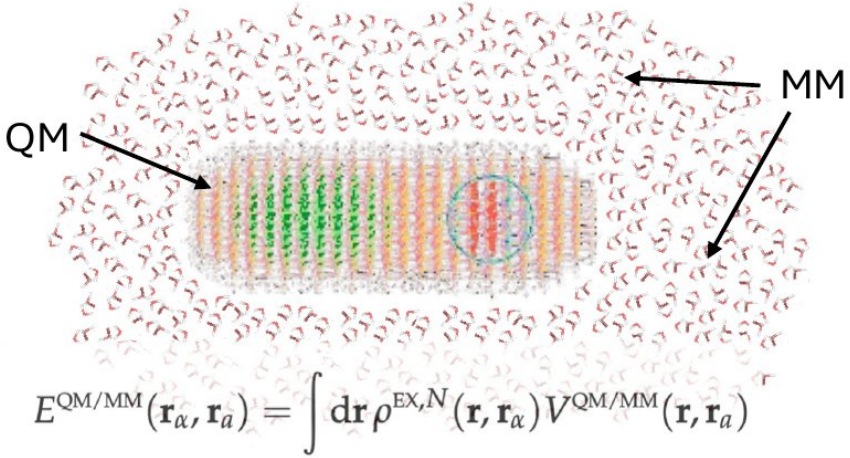
Anisotropic electrostatic
GFN2-xTB
$E_{\text{elec}}^{\text{GFN2-xTB}} = E_{qq} + E_{q\mu} + E_{q\theta} + E_{\mu\mu}$

Isotropic electrostatic
GFN1-xTB
$E_{\text{elec}}^{\text{GFN1-xTB}} = E_{qq}$

Multipole correction for sTDA
$\Omega^{\text{sTDAcorr}} = \Omega^{\text{sTDA}} + \sum_A \left[\frac{2}{3\sqrt{\Pi}} \eta_A^3 |\boldsymbol{\mu}^A|^2 + \frac{8}{45\sqrt{\Pi}} \eta_A^5 \text{Tr}|\mathbf{Q}^A|^2 \right]$

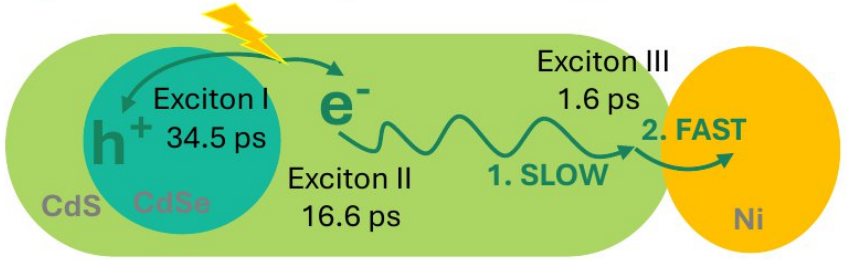
120 nm size range of GFN1-xTB

2. and their surrounding environment

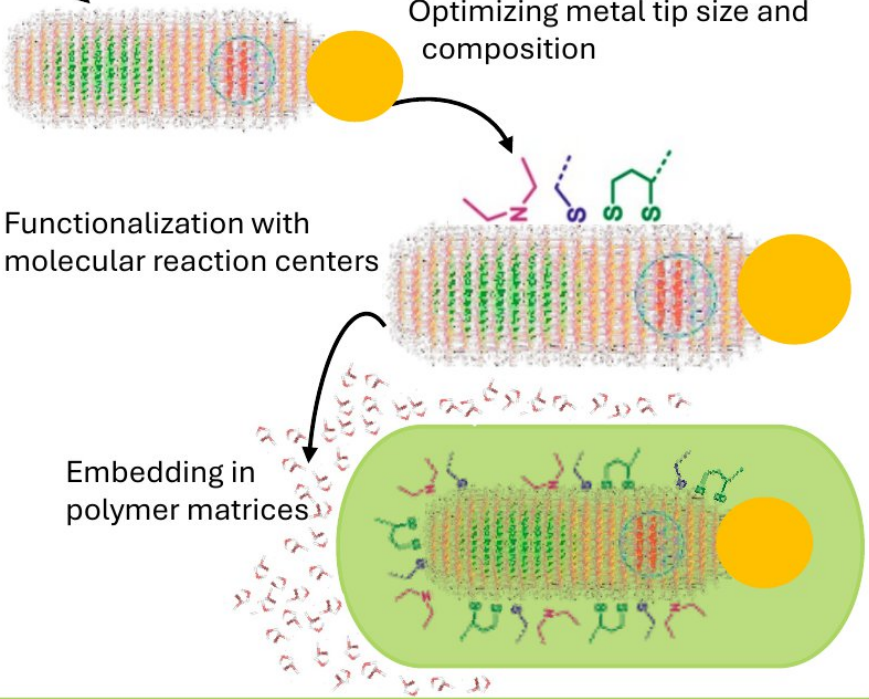


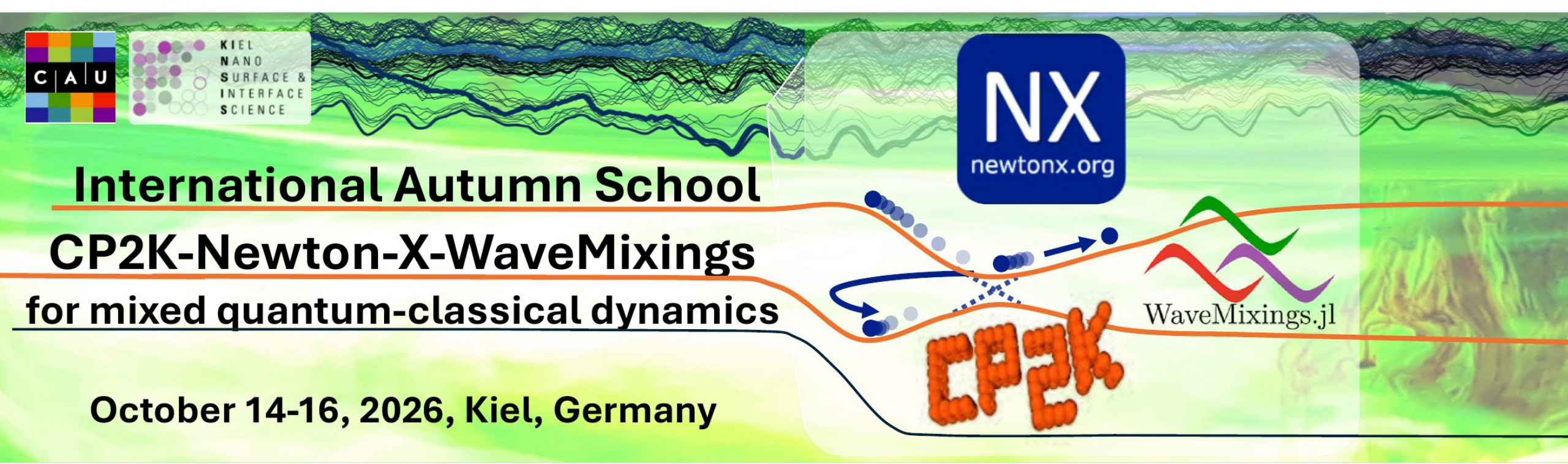
$$E^{\text{QM/MM}}(\mathbf{r}_\alpha, \mathbf{r}_a) = \int \mathrm{d}\mathbf{r}\, \rho^{\text{EX},N}(\mathbf{r}, \mathbf{r}_\alpha) V^{\text{QM/MM}}(\mathbf{r}, \mathbf{r}_a)$$

Modeling charge carrier and reaction dynamics with QM/MM setup



3. to assess current experimental strategies with the aim to increase photocatalytic performance for water splitting





International Autumn School

CP2K-Newton-X-WaveMixings

for mixed quantum-classical dynamics

October 14-16, 2026, Kiel, Germany

Contributions by Mario Barbatti, Ritama Kar, Rafael Souza-Mattos (Marseille)
Maxim Gelin, Luis Vasquez (Hangzhou Dianzi, China)
Stepan Marek (Group of Jan Wilhelm, Regensburg)
Philipp Schienbein (Bochum)
Anna Hehn, Tejas Thorat (Kiel)

Webpage https://github.com/SPECATgroup/CP2Kautumnschool.github.io

Event site Wissenschaftszentrum, Fraunhoferstraße 13, 24118 Kiel, Germany

Funding by Internationalisation Funds of the CAU: will be used to finance travel costs of lecturers / participants

International Autumn School

CP2K-Newton-X-WaveMixings

for mixed quantum-classical dynamics

October 14-16, 2026, Kiel, Germany

Contributions by Mario Barbatti, Ritama Kar, Rafael Souza-Mattos (Marseille)
Maxim Gelin, Luis Vasquez (Hangzhou Dianzi, China)
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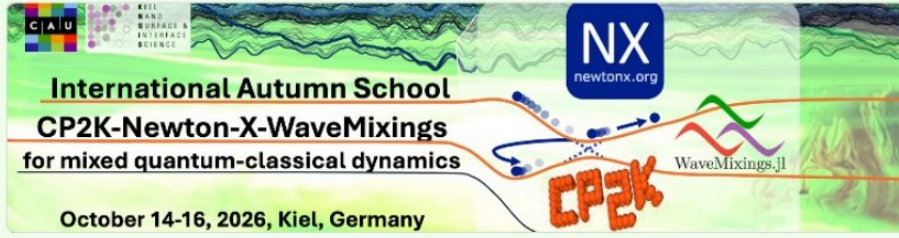
Registration will open asap ->



CP2K-Newton-X autumn school registration form

Event Timing: October 14th-16th, 2026
Event Address: Wissenschaftszentrum Kiel, Fraunhoferstraße 13, 24118 Kiel, Germany

Name *

Short answer text

Email *

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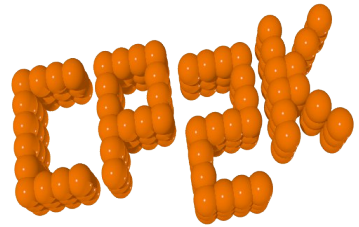
Missing contributions?

Thank you to all new contributors!

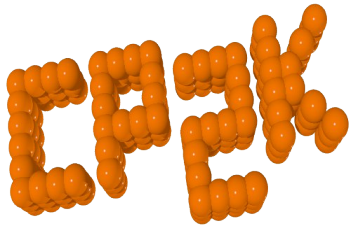
Current Issues with CP2K

- Default block size is too small (64). What about increasing it to 256? (https://manual.cp2k.org/trunk/CP2K_INPUT/GLOBAL/FM.html)
  - Last time: larger block size problematic for benchmark tests
  - 128 instead? different block sizes depending on the hardware/software?
- The Cholesky decomposition is sometimes computed without being needed. (context: libraries with generalized eigenvalue solvers)
  - Artefact from refactoring generalized eigenvalue problems
  - needs further investigations
  - removal may lead to substantial reduction in compute time



Next CP2K Release

- Early July



Planned Events in the Context of CP2K

- Past:
  - International Autumn School on CP2K-GROMACS for Multiscale Atomistic Simulation, (Sept. 29 - Oct.1, 2025 PC2 in Paderborn)

  https://events.uni-paderborn.de/event/797/
- Planned:
  - Quickstep to the Future, 25 Years of CP2K, (June 17-19, 2026 Zürich) https://www.cp2k.org/news:common:index
  - International Autumn School CP2K-Newton-X-WaveMixings for mixed quantum-classical dynamics (Oct. 14-16, 2026, Kiel) https://github.com/SPECATgroup/CP2Kautumnschool.github.io

Other interesting events:

– Atomic Simulation Environment: Mainz, June 15-19 (Johann Pototschnig and Vahidev Alizadeh)

– Wannier90 Developers Meeting: Trieste, September 7-11

– ReLibQC 2026 Workshop on Reusable Libraries for Quantum Chemistry in Toulouse, France, Sep 21-24 2026, https://relibqc.github.io/

CP2K Beginner Workshops

How to proceed?

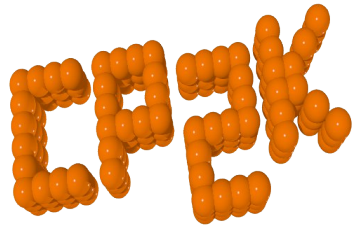
Who would be interested?

Set up a separate meeting?

Not only using but also compiling CP2K

CP2K Lab

Note: conda is working again



Open Discussion: Compiling and Dependencies

- Spack (mainly for HPC), Conda (mainly for client systems)
- Dependency management
- growing the developer community
- handling/removal of legacy/unmaintained dependencies
- option for a freeze period or other methods

Benchmarks:

– https://benchmarks-max3-max-centre-9958bb5003607b47e1a11ae4c1cc8cae2cd0.gitlab.io/qe.html