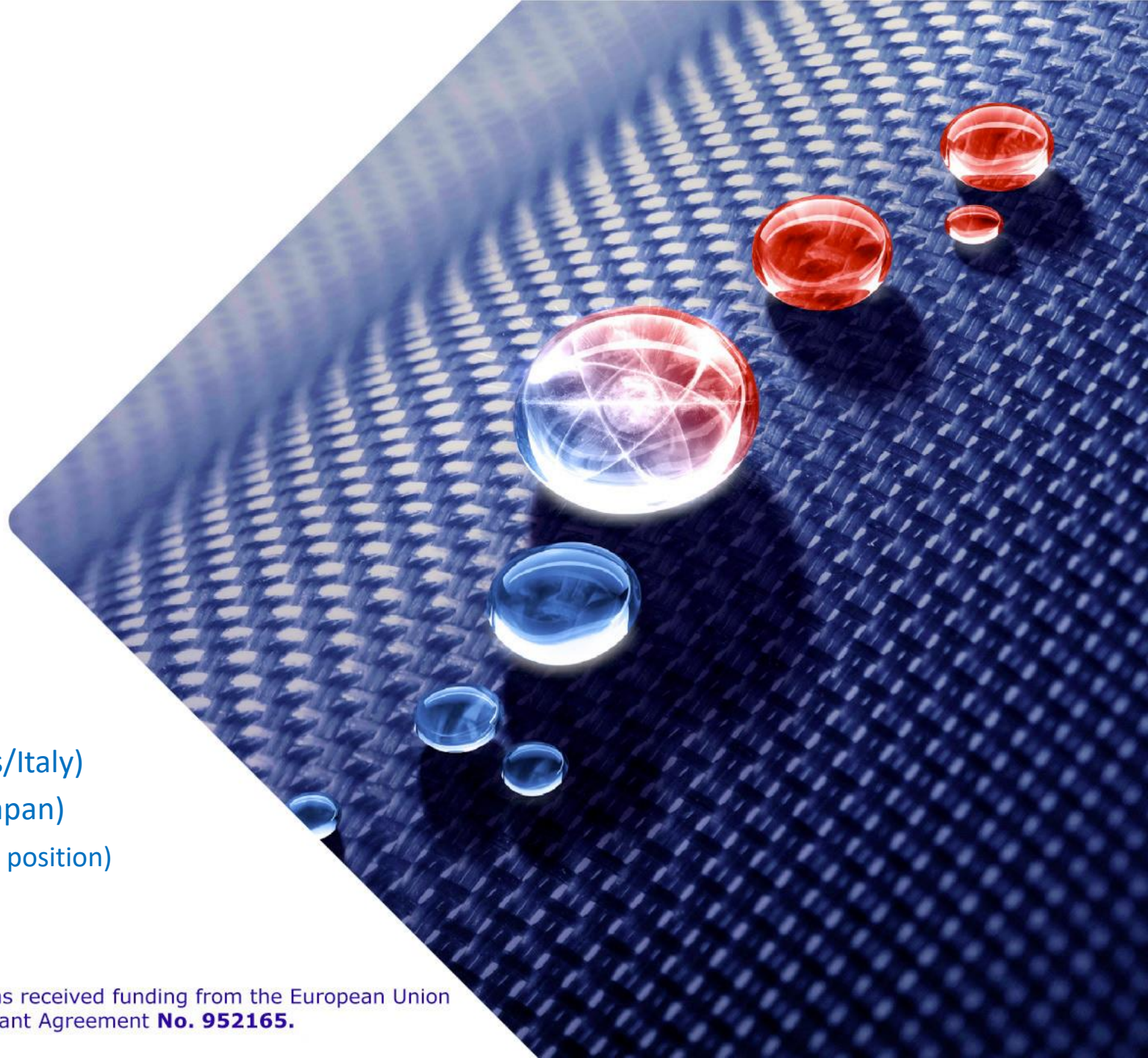
Targeting Real chemical accuracy at the EXascale

TurboRVB and TurboWorkflows



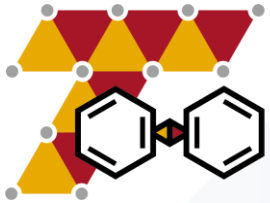
Kosuke Nakano

- SISSA (International School for Advanced Studies/Italy)
- NIMS (National Institute for Materials Science/Japan)

(Current position)

Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizon 2020 research and innovation programme under Grant Agreement **No. 952165.**

Packages: TurboRVB and TurboWorkflows



TurboRVB
Quantum Monte Carlo Package SISSA

QMC engines (DFT, VMC, and DMC).

K. Nakano, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula, E. Coccia, M. Dagrada, Y. Luo, G. Mazzola, A. Zen, and S. Sorella, ***J. Chem. Phys.*** 152, 204121 (2020)

TurboGenius

Command line tools (python).

Turbo Workflows

Workflow systems (python).

K. Nakano et al., ***in preparation*** (2023)

TurboRVB Features

TurboRVB Quantum Monte Carlo Package SISSA

The main developer was Prof. Sandro Sorella.

The project PIs are M. Casula and K. Nakano.

open-source by July 2023!!

- Variational Monte Carlo (VMC) and Lattice regularized Diffusion Monte Carlo (LRDMC).

M. Casula et al., ***Phys. Rev. Lett*** 95, 100201 (2005)

- Atomic Forces by exploiting the algorithmic differentiation (AD).

S. Sorella et al., ***J. Chem. Phys.*** 133, 234111 (2010)

- Flexible ansatz such as Antisymmetrized Geminal Power (AGP) and Pfaffian (Pf).

M. Casula et al., ***J. Chem. Phys. 119***, 6500 (2003)

C. Genovese et al., ***J. Chem. Theory Comput.*** 16, 6114 (2020)

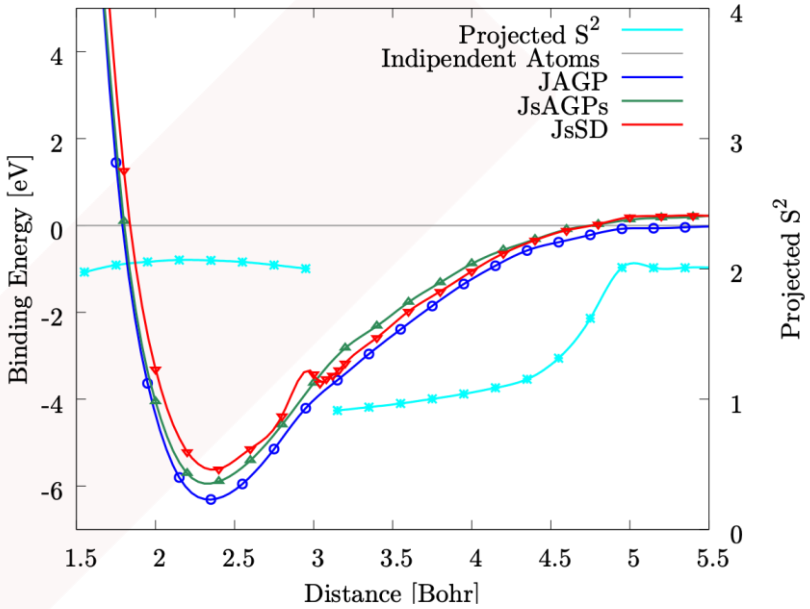
- Parallelized by MPI/OpenMP (hybrid) and GPU.

O. Kohulak et al., in prerаration (2023)

Example: Potential Energy Surface: C_2-dimer

Binding energies of the C_2 dimer obtained by LRDMC

Wavefunction	C atom (Ha)	C_2 molecule (Ha)	Binding (eV)
Jastrow Slater	−37.82966(4)	−75.8672(1)	5.656(3)
Jastrow Geminal (Singlet)	−37.8364(1)	−75.8938(2)	6.01(1)
Jastrow Geminal (Singlet + broken sym.)	−37.8364(1)	−75.8935(2)	6.00(1)
Jastrow Geminal (All-pairing, Pfaffian)	− 37.8363(1)	−75.9045(2)	**6.31(1)**
Estimated exact	-37.8450	−75.9045(2)	6.44(2) (Exp.)



More complex ansatz.

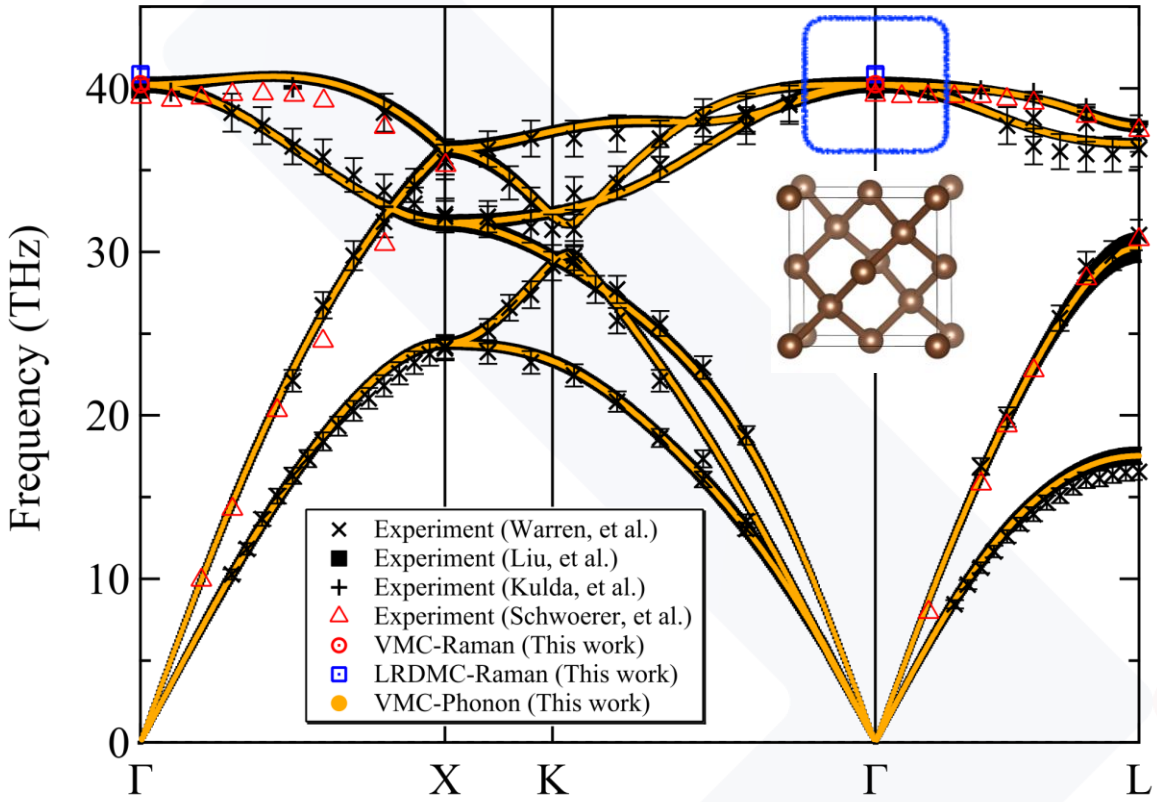
C. Genovese et al., ***J. Chem. Theory Comput.*** 16, 6114 (2020)

DMC gives a more accurate result than CCSD(T) does for the challenging molecule.

Example: Phonon dispersion of Diamond

- Diamond: the conventional 2x2x2 supercell with the experimental lattice parameter
- Employed the frozen phonon method implemented in Phonopy package.

A. Togo and I. Tanaka, *Scr. Mater.* 108, 1 (2015).



* including anharmonic corrections.

Raman Freq. (optical phonon at Γ)

DFT-LDA	38.55 THz
VMC	40.65(38) THz
Exp.	40.35 THz

** These are harmonic frequencies

K. Nakano *et al.*, ***Phys. Rev. B*** 103, L121110 (2021)

TurboWorkflows Features

- Controlling QMC jobs on a python script

```
vmcopt_workflow = eWorkflow(
    label=f'vmcopt-workflow',
    dirname=f'vmcopt-workflow',
    input_files=[Variable(label=f'trexio-workflow', vtype='file', name='fort.10'),
                 Variable(label=f'trexio-workflow', vtype='file', name='pseudo.dat')],
    workflow=VMCopt_workflow(
        ## job
        server_machine_name="fugaku",
        cores=48,
        openmp=1,
        queue="small",
        version="stable",
        sleep_time=180,
        ## vmcopt
        vmcopt_max_continuation=2,
        vmcopt_target_error_bar=1.0e-3, # Ha
        vmcopt_trial_optsteps=50,
        vmcopt_trial_steps=50,
        vmcopt_production_optsteps=20,
        vmcopt_optwarmupsteps_ratio=0.8,
        vmcopt_bin_block=1,
        vmcopt_warmupblocks=0,
        vmcopt_optimizer="lr",
        vmcopt_learning_rate=0.35,
        vmcopt_regularization=0.001,
        vmcopt_onebody=True,
        vmcopt_twobody=True,
        vmcopt_det_mat=False,
        vmcopt_jas_mat=True,
        vmcopt_det_basis_exp=False,
        vmcopt_jas_basis_exp=False,
```

https://github.com/kousuke-nakano/turboworkflows

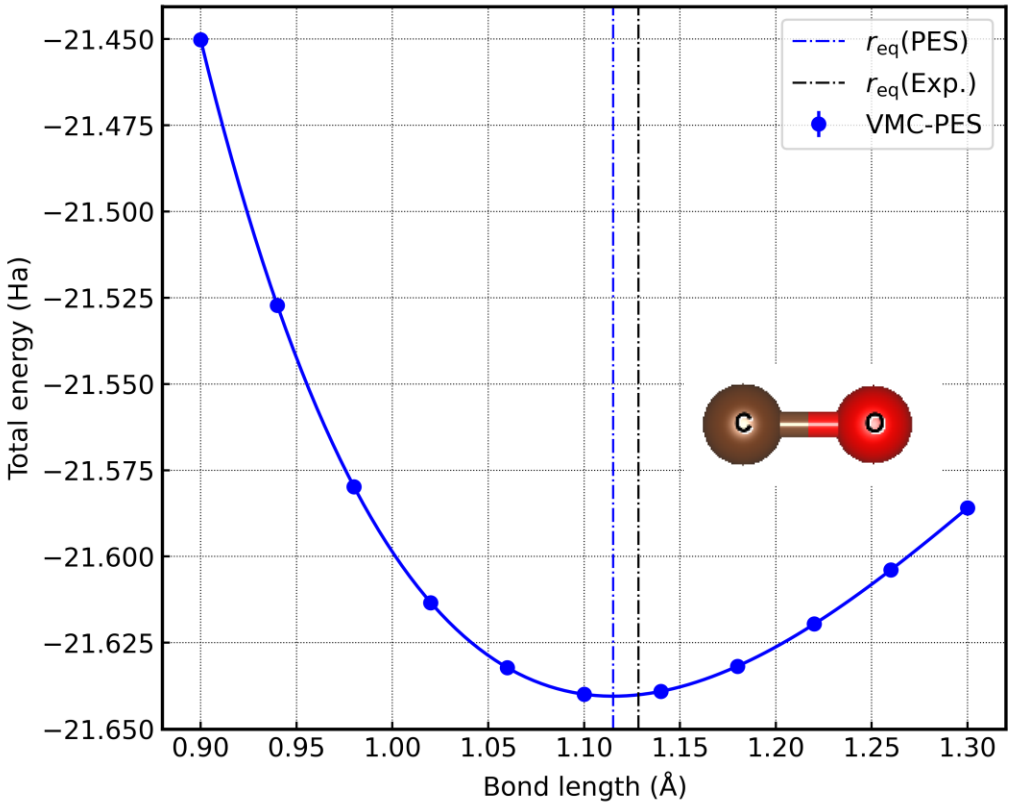
Turbo Workflows

In production from 2022 -

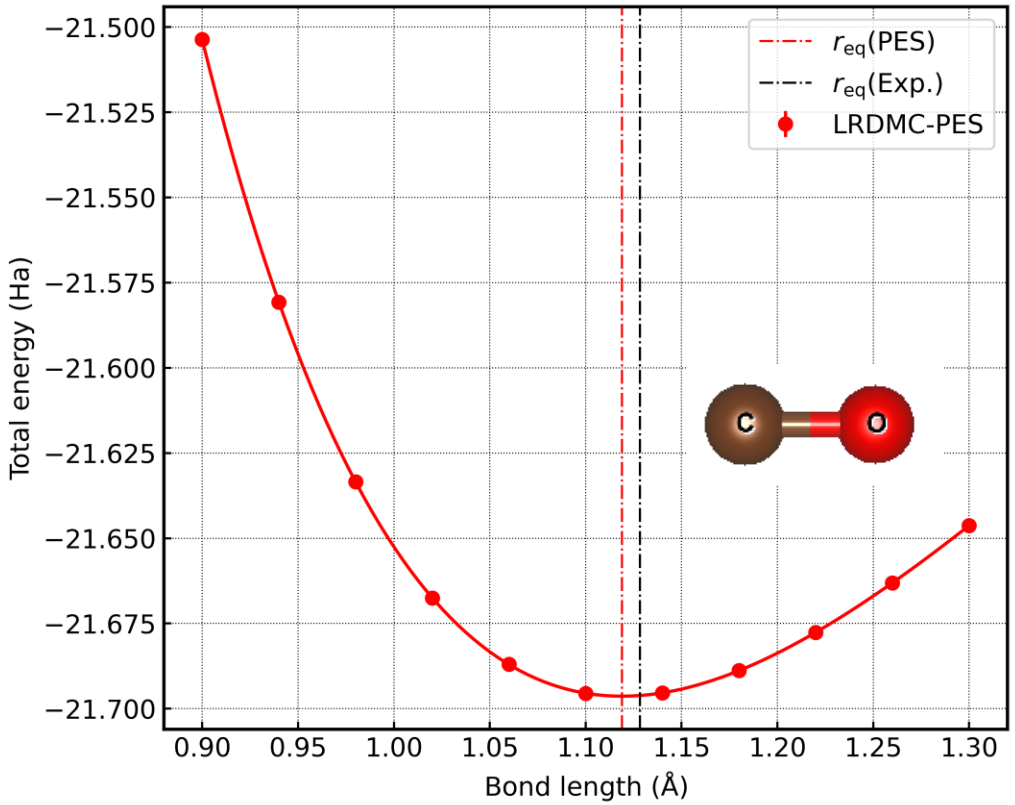
- Implemented in object-oriented fashion by Python3
- Solving dependencies and monitoring jobs
- Allowed to define user's own workflows
- Open source under the BSD3 license (Jul. 2023-)

K. Nakano *et al*., in preparation (2023)

TurboWorkflows Example: Pontential Energy Surface of CO



PES at the VMC level.



PES at the LRDMC level.

TurboWorkflows Example: Pontential Energy Surface of CO

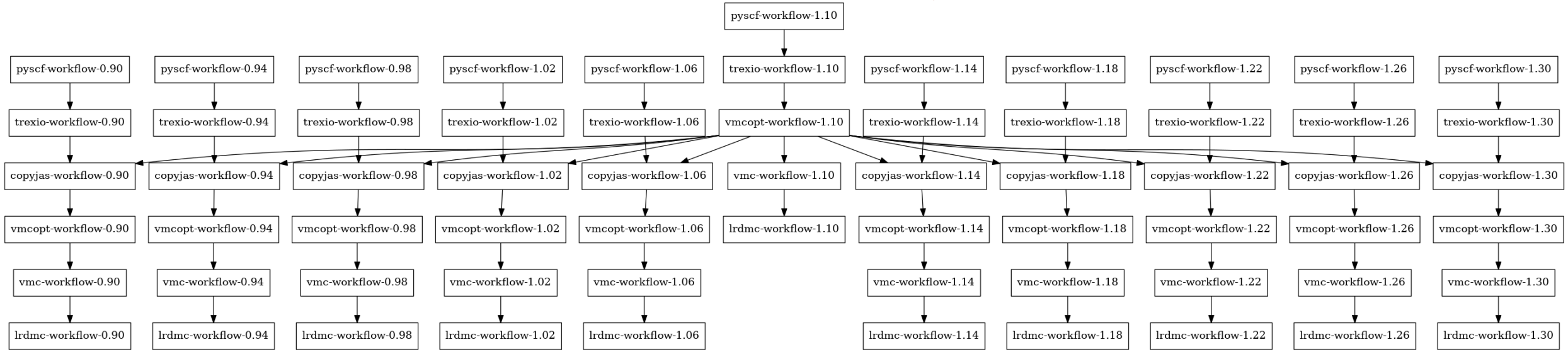
```
vmcopt_workflow = eWorkflow(
    label=f'vmcopt-workflow',
    dirname=f'vmcopt-workflow',
    input_files=[Variable(label=f'trexio-workflow', vtype='file', name='fort.10'),
                 Variable(label=f'trexio-workflow', vtype='file', name='pseudo.dat')],
    workflow=VMCopt_workflow(
        ## job
        server_machine_name="fugaku",
        cores=48,
        openmp=1,
        queue="small",
        version="stable",
```

A python script defining the QMC workflows.

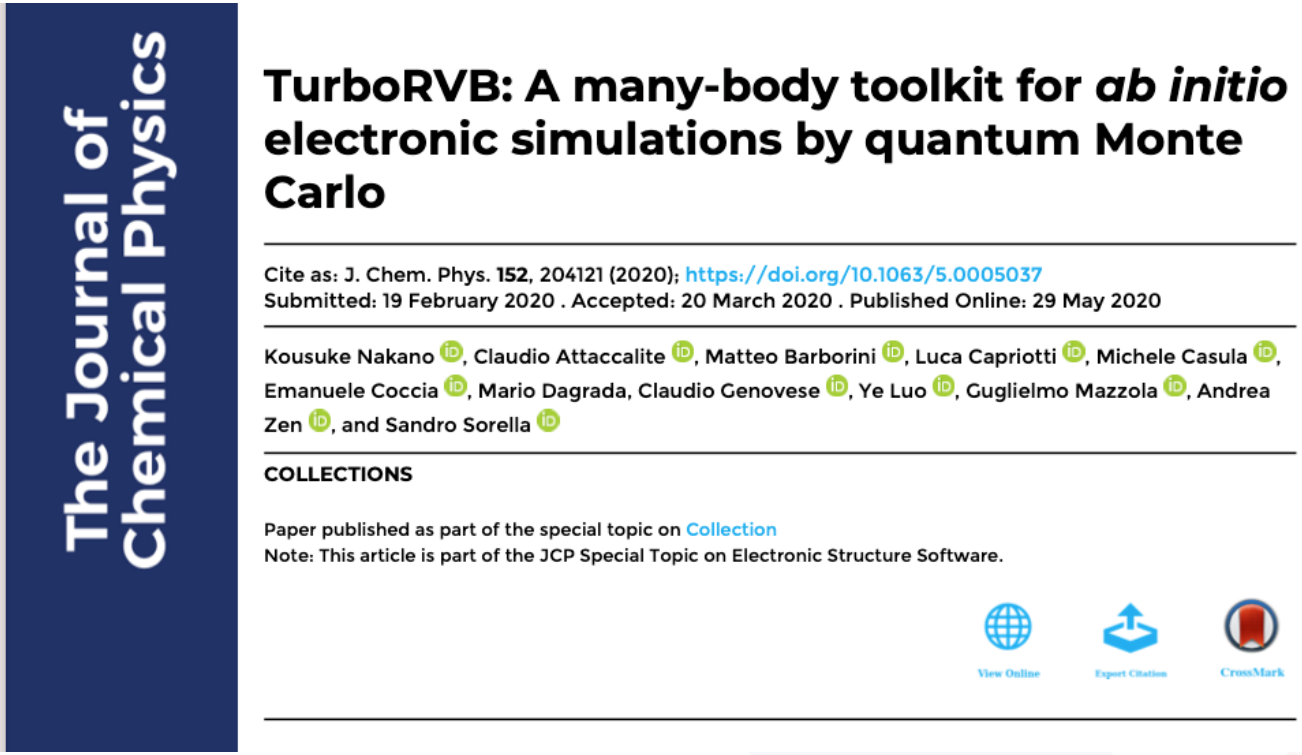
with TREXIO

Turbo Workflows

It automatically solves the dependencies of the calculations.



Review and Website


The Journal of Chemical Physics

TurboRVB: A many-body toolkit for *ab initio* electronic simulations by quantum Monte Carlo

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COLLECTIONS

Paper published as part of the special topic on Collection
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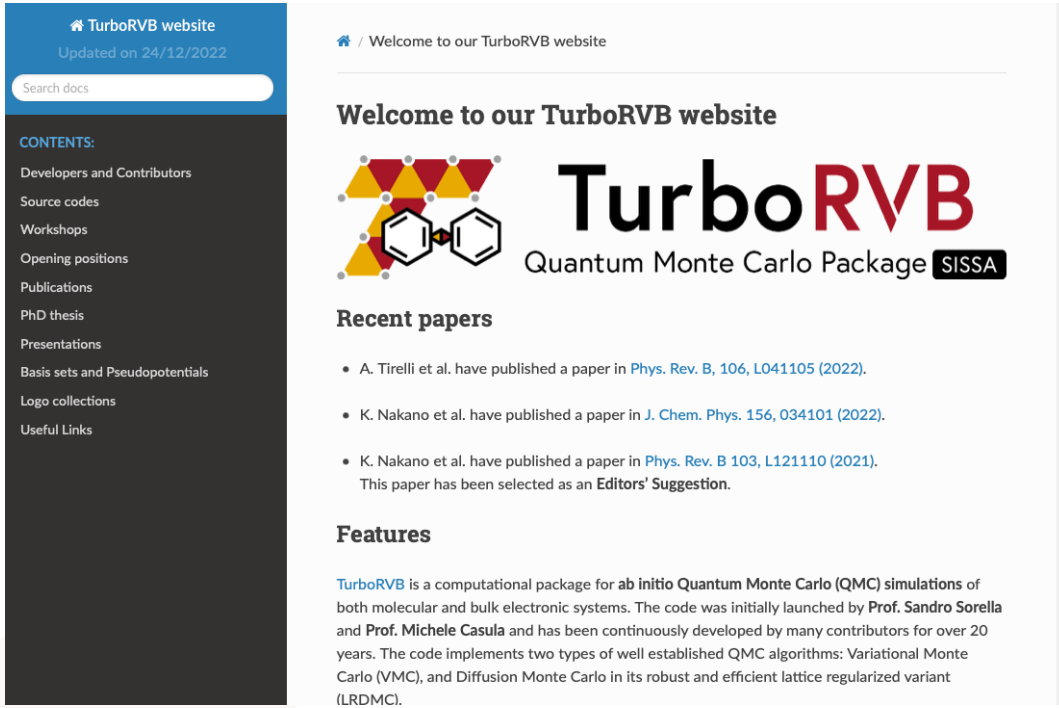
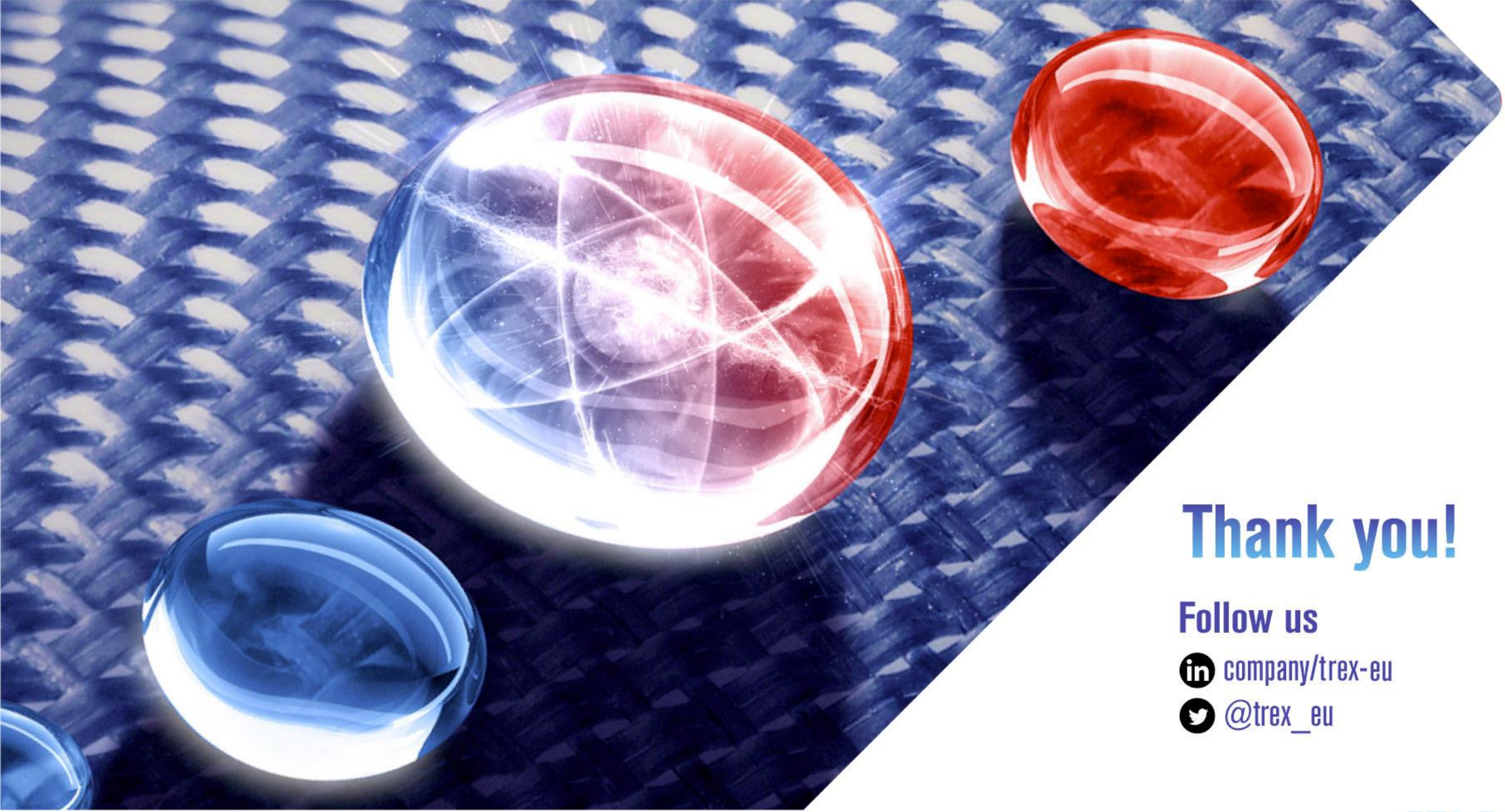


https://turborvb.sissa.it

K. Nakano, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula, E. Coccia, M. Dagrada, Y. Luo, G. Mazzola, A. Zen, and S. Sorella, ***J. Chem. Phys.*** 152, 204121 (2020)



Thank you!

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