Schedule Literature Seminar

The seminar takes place in our group room (HCI G 232) at 2 p.m.

Topic	Article	Person in charge	Introduction	Discussion
MC-PDFT	[1]	Vera	Feb. 20	Feb. 27
Machine-learning CC	[2]	Christoph	Mar. 20	Mar. 27
Exact factorization of the electron-nuclear wave function	[3]	Andrea	April 3	April 10
FCIQMC	[4]	Alberto	May 15	May 29

References

[1] Li Manni, G., Carlson, R. K., Luo, S., Ma, D., Olsen, J., Truhlar, D. G., Gagliardi, L., Multiconfiguration Pair-Density Functional Theory, *J. Chem. Theory Comput.*, **10**(9) (2014) 3669–3680.

[2] Margraf, J. T., Reuter, K., Making the Coupled Cluster Correlation Energy Machine-Learnable, *J. Phys. Chem. A*, **122**(30) (2018) 6343–6348.

[3] Scherrer, A., Agostini, F., Sebastiani, D., Gross, E. K. U., Vuilleumier, R., On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation, *Phys. Rev. X*, **7**(3) (2017) 031035.

[4] Booth, G. H., Thom, A. J. W., Alavi, A., Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space, *J. Chem. Phys.*, **131**(5) (2009) 054106.