

Can we treat the dynamics of electronic correlations, both accurately and efficiently?

Monday 12 September 2022 11:30 (45 minutes)

Electronic correlations –Coulomb interaction effects beyond the simple mean field –are crucial for the correct description of warm dense matter. Moreover, correlations are responsible for scattering effects, including Auger-type processes, multiple excitations and so on. When the system is driven out of equilibrium, correlations are strongly modified and undergo their own dynamics [1]. While such processes are difficult to capture with DFT approaches, a systematic treatment of the dynamics of electronic correlations is possible with nonequilibrium Green functions (NEGF) that we have been developing over the past decades. I will give an overview on recent progress in achieving higher accuracy and dramatically speeding up the expensive simulations [2, 3]. I will conclude by presenting first results for the dynamics of electrons in warm dense matter and outline how to bridge the gap from very short to macroscopic times.

[1] A. Niggas et al., Phys. Rev. Lett. 129, 086802 (2022)

[2] N. Schlünzen et al., Phys. Rev. Lett. 124, 076601 (2020)

[3] J.-P. Joost et al., Phys. Rev. B 105 (16), 165155 (2022)

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Session Classification: Morning Session (Monday)