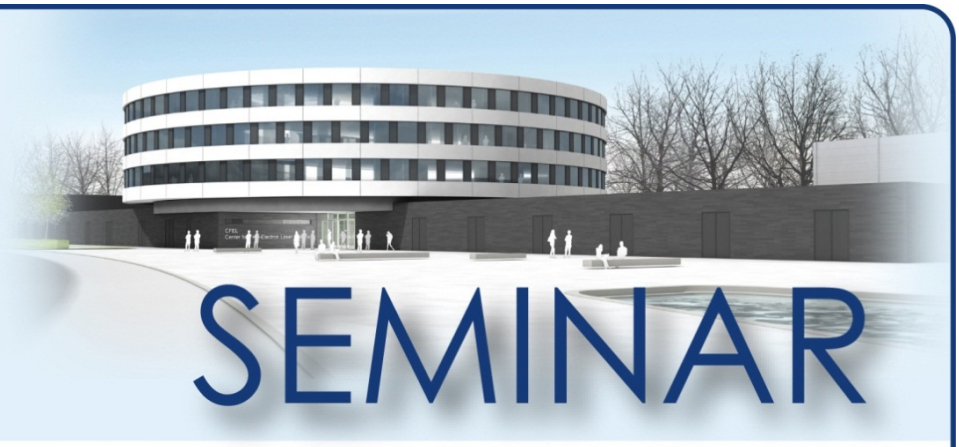
CFEL SCIENCE



SEMINAR

6th March 2024 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Deep-learning approach for the atomic configuration interaction problem on large basis sets

In atomic structure computations, accurate modeling of many-electron correlations is typically achieved by a multiconfiguration expansion of the electronic wave function to be found. Unfortunately, high precision demands imposed on the obtained atomic data often lead to infeasibly large expansions even for advanced parallelized codes running on supercomputer systems. Often, however, only a small part of this basis is essential and the rest could be discarded without considerable harm to the quality of the obtained results. We present a deep-learning approach [1], which allows to identify the essential basis part and extend it iteratively until the required energy precision is achieved. In one iteration, an approximative basis set is first formed from a neural-network prediction, and then forwarded to the atomic code for diagonalization. The results are then used in neural network retraining for the next iteration. We demonstrate the approach both on a moderate basis allowing for a direct computation, and a basis of a huge size ruling out such possibility.

[1] P. Bilous, A. Pálffy, and F. Marquardt, *Phys. Rev. Lett.* **131**, 133002 (2023).

Host: Robin Santra – CFEL-DESY Theory Division