CFEL SCIENCE

SEMINAR

16th January 2019 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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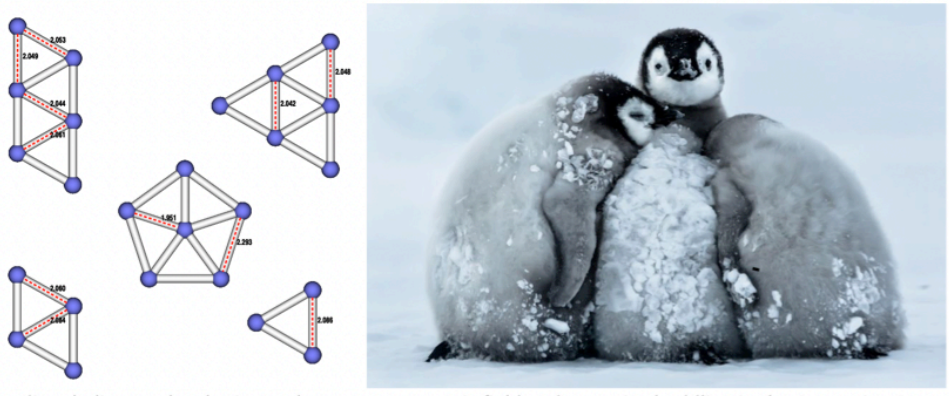
Chemistry in a strong magnetic field

In a strong magnetic field, chemistry changes: electronic states change their character, atoms and molecules change their shape, and their interactions with radiation are affected, often in a dramatic manner. Perhaps most surprisingly, new bonding mechanisms occur, giving rise to molecules that do not exist on Earth but may exist elsewhere such as in the atmospheres of magnetic white dwarfs. The exotic chemistry of atoms and molecules in strong magnetic fields provides a fresh perspective on the familiar chemistry on Earth; at the same time, it provides a stress test for quantum chemistry, whose methods have been developed for Earth-like conditions. Density-functional theory, for example, must be re-examined and adapted for the molecules in strong magnetic fields and such modifications have relevance also for the calculation of magnetic properties such as shielding constants and magnetizabilities.

In the talk, I give an overview of chemistry in strong magnetic fields and discuss the how the methods of quantum chemistry such as coupled-cluster theory and density-functional theory must be modified and adapted to study molecules and their electronic structure in magnetic fields.



Bonding: helium molecules in an ultrastrong magnetic field and penguins huddling in the Antarctic winter

Host: Robin Santra – CFEL-DESY Theory Division