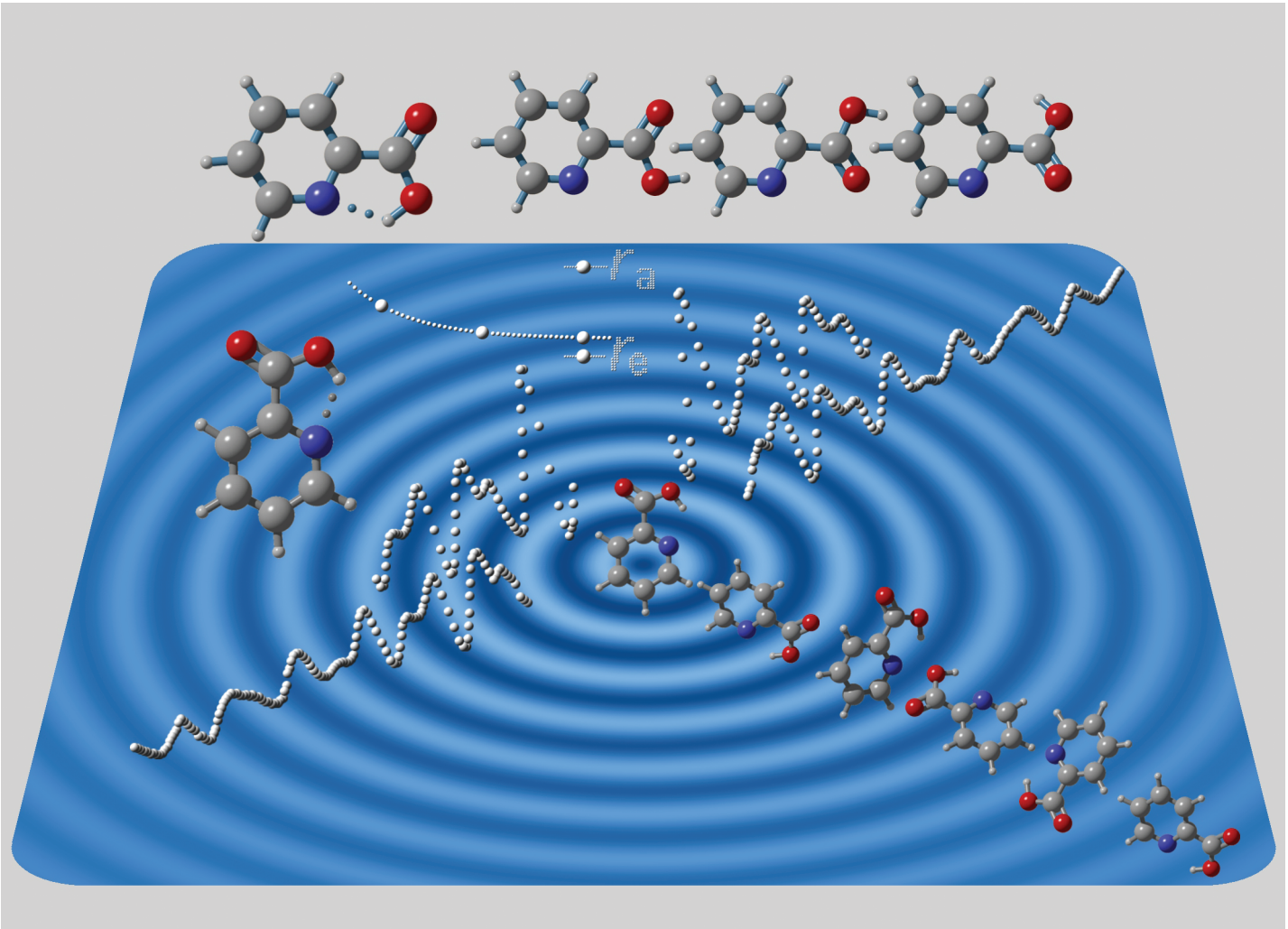

Showcasing research by the group of Prof. Dr Natalja Vogt at the Section of Chemical Information Systems of the University of Ulm (Germany) and the Chemistry Department of the Lomonosov Moscow State University (Russia)

Experiment and theory at the convergence limit: accurate equilibrium structure of picolinic acid by gas-phase electron diffraction and coupled-cluster computations

This work presents comprehensive studies of molecular structures benchmarking both experiment and theory. A remarkable agreement between the experimental and computed structures of picolinic acid is reached by taking into account anharmonic vibrational effects and increasing the level of computations (up to CCSD(T)_ae/cc-pwCVQZ), respectively. High accuracy equilibrium structures of the picolinic acid conformers and pyridine, exploited for the observation of mesomeric effects and influence of hydrogen bonds, deliver contributions to structural chemistry.

As featured in:

See Natalja Vogt *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 9787.

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