GDCh

Gesellschaft Deutscher Chemiker
Ortsverband Hannover

Einladung zum GDCh-Colloquium des Ortsverbandes Hannover

SONDERTERMIN: Das Colloquium findet um 16c.t. im Dr.-Oetker Hörsaal (Raum 007, Geb. 2504) der Leibniz Universität Hannover, Physikalische Chemie, Callinstraße 3A, 30167 Hannover statt.

Montag, 13.07.2026

Prof. Dr. John Herbert,
The Ohio State University, Columbus, OH

High-Fidelity Fragmentation Methods for Enzymatic Quantum Chemistry

Fragment-based methods offer a promising way to defeat the nonlinear scaling of conventional quantum chemistry by means of distributed computing, and thereby extend electronic structure calculations to large molecular systems including enzymatic reactions and protein–ligand binding. At present, quantum chemistry calculations in those domains are limited to mixed quantum/classical (QM/MM) methods whose convergence is very slow with respect to the size of the QM region. Typical QM system sizes (50–100 atoms) may yield the wrong sign for enthalpy changes, and selection of an appropriate QM region must be pinned to experimental data and often rests on error cancellation. This talk will describe methods that can be used to obtain converged results at the *ab initio* limit (including methods beyond density functional theory), in an affordable manner on research-group-scale hardware.

Prof. Dr. Jens-Uwe Grabow
Vorsitz OV Hannover

Vor dem Colloquium findet ab ca. 15:30. eine ‚Kaffeerunde' mit dem Vortragenden in der Bibliothek des Instituts für Physikalische Chemie, Callinstraße 3A statt.