

# Turbomole: Today and Tomorrow

16<sup>th</sup>-19<sup>th</sup> September 2024

St Hilda's College, Cowley Road, Oxford

Tuesday 17<sup>th</sup> Sept : Jacqueline du Pre Building

08:00	Breakfast : self-service in dining hall
09:00	Eva Von Domaros - <i>Gaining new insights: nuclei in electronic structure calculations</i>
09:35	Christof Holze - <i>Light-matter interactions and beyond: From molecules to materials</i>
10:05	Ritaj Tyagi - <i>Anionic states using single-pole polarization potentials</i>
10:30	Coffee
11:00	David Waroquier - <i>How to streamline TURBOMOLE simulations?</i>
11:35	Pulkit Joshi - <i>Beyond-RPA corrections for open-shell intermolecular interactions</i>
12:00	Lunch : self-service in dining hall

Wednesday 18<sup>th</sup> Sept : Jacqueline du Pre Building

08:00	Breakfast : self-service in dining hall
09:00	Marek Sierka - <i>Materials simulations with the Ripex module</i>
09:35	Dimitrij Rappoport - <i>Density functional studies at the intersection of electronic and vibrational properties</i>
10:05	Arman Nejad - <i>Progress report on a 3D-periodic PNO-MP2 implementation in TURBOMOLE</i>
10:30	Coffee
11:00	David Tew - <i>Low-scaling explicitly-correlated coupled-cluster methods in TURBOMOLE</i>
11:35	Shane Parker - <i>TDDFT-ris: A semiempirical model and preconditioner for fast and accurate spectra and nonlinear properties</i>
12:05	Lunch : self-service in dining hall

Thursday 19<sup>th</sup> Sept : Jacqueline du Pre Building

08:00	Breakfast : self-service in dining hall
09:00	Ansgar Pausch - <i>From Solvation to High Pressure: Molecules and their Environments</i>
09:35	Christof van Wüllen - <i>Towards the calculation of iridium Moessbauer parameters</i>
10:05	Manas Sharma - <i>Density functional theory-based embedding for periodic systems using gaussian basis functions</i>
10:30	Coffee

# Conference Schedule

Monday 16<sup>th</sup> Sept: Riverside Pavilion

16:00	Registration
18:00	Stefan Grimme - <i>Automated Quantum Chemistry Workflows</i>
19:00	Buffet dinner

12:00	Lunch : self-service in dining hall
14:00	Antti Karttunen - <i>Anharmonic phonon properties with TURBOMOLE and ALAMODE</i>
14:35	Uwe Huniar - <i>TURBOMOLE Tomorrow: "Tools not Toys" Reloaded</i>
15:00	Fabian Pauly - <i>Charge and heat transport through nanojunctions</i>
15:30	Coffee
16:00	Kshatresh Dutta Dubey
16:35	Rahul Kumar Jadav - <i>Engineering MBene-terminated anodes for improved post-Li/Ca-ion battery efficiency</i>
19:00	Conference dinner in the Pavilion

12:05	Lunch : self-service in dining hall
14:00	Christof Hättig - <i>Recent developments for including solvent effects in ADC(2) and CC2 calculations</i>
14:35	Anja Appenzeller - <i>From magnetic circular dichroism spectroscopy to magnetic white dwarfs: TURBOMOLE's toolset for finite magnetic fields</i>
15:00	Martijn Zwijnenburg - <i>Predicting the electronic and optical properties of inorganic nanoparticles</i>
15:30	Coffee
16:00	Florian Weigend - <i>Quasi-relativistic electronic structure theory: Recent developments and applications</i>
16:35	Yannick Franzke - <i>Relativistic Methods for NMR/EPR Spectroscopy and Beyond: "Tools not Toys"</i>
17:05	Dominik Steinmetz - <i>The Berry curvature in finite magnetic fields and its relevance in rovibrational spectroscopy</i>
19:00	Poster session and buffet dinner

10:30	Coffee
11:00	Vamsee Voora - <i>High-performance polarization models for charged-excitations in matter</i>
11:35	Michael Harding - <i>Basis functions with angular momentum greater than <math>l</math> with TURBOMOLE</i>
12:05	Niklas Sülzner - <i>Going beyond implicit solvent effects on hydroxypyrene photoacids</i>
12:30	Lunch : self-service in dining hall