



Institute/Department	Acronym	Group Leaders	Web Page	
College of Chemistry and Chemical Engineering	PCC	Pavlo O. Dral	http://dr-dral.com	
METHODOLOGY				
General keyword	Details in topic	Researchers involved	Institute (Group Acronym)	
machine learning; semiempirical molecular orbital methods	Machine learning quantum chemical properties. Machine-learning-enhanced quantum chemical methods	Pavlo O. Dral	XMU (PCC)	
open quantum systems, quantum dissipative dynamics, spin-boson system	Quantum dissipative dynamics of open systems	Arif Ullah		
APPLICATIONS				
Systems	Property	Methods	Researchers involved	Institute (Group Acronym)
mostly organic molecules	reaction energies and mechanisms, thermochemistry, accurate geometries, electronic spectra, IR spectra, aromaticity	ML, semiempirical molecular orbital methods, DFT, CCSD(T), trajectory surface hopping	Assoc. Prof. Pavlo O. Dral	XMU (PCC)
light-harvesting systems	time evolution of electronic state populations	hierarchical equations of motions, stochastic equations of motion, machine learning	Dr. Arif Ullah	