

Day I: Monday June 30		
7:30-8:45		Registration (ENSCR Entrance Hall)
8:45-9:00		Welcome
9:00-10:30	Marie-Therese Hübsch	Introduction to ab-initio simulations with VASP (DFT, PAW, basic input)
10:30-11:00		Coffee break
11:00-12:30	Fabien Tran	Electronic relaxation, sampling reciprocal space and Wannierization
12:30-14:30		Lunch (Marie Curie - ENSCR)
14:30-18:00	(30 min break)	Exercises I: Atoms, molecules and simple bulk
18:00-20:30		Poster session & buffet (Marie Curie - ENSCR)
Day II: Tuesday, July 1		
9:00-10:30	Manuel Engel	Ionic relaxation, pressure, data analysis and visualization using py4vasp
10:30-11:00		Coffee break
11:00-12:30	Marie-Therese Hübsch	Basics of MD and MLFF
12:30-14:30		Lunch (Marie Curie - ENSCR)
14:30-18:00	(30 min break)	Exercises II: MD and MLFF
Day III: Wednesday, July 2		
9:00-10:30	Xavier Rocquefelte	The spin degrees of freedom (collinear magnetism)
10:30-11:00		Coffee break
11:00-12:30	Marie-Therese Hübsch	Spin waves, noncollinear magnetism and spin-orbit coupling
12:30-14:30		Lunch (Marie Curie - ENSCR)
14:30-18:00	(30 min break)	Exercises III: Magnetism
19:30		Gala dinner
Day IV: Thursday, July 3		
9:00-10:30	Manuel Engel	Harmonic and anharmonic phonons
10:30-11:00		Coffee break
11:00-12:30	Manuel Engel	Electron-phonon coupling with a focus on transport properties
12:30-14:30		Lunch (Marie Curie - ENSCR)
14:30-18:00	(30 min break)	Exercises IV: Phonons and electron-phonon coupling
Day V: Friday, July 4		
9:00-9:45	Fabien Tran	Exchange-correlation effects revisited (MGGA, hybrids, HF, MBPT)
9:45-10:30	Manuel Engel	Running VASP efficiently
10:30-11:00		Coffee break
11:00-12:30		Exercises V: Hybrid functionals
12:30-14:30		Lunch (Marie Curie - ENSCR)
14:30-...		<i>Round table (feedback)</i>
		Closing