

Day I: Monday June 30			
7:30-8:45		Registration (ENSCR Entrance Hall)	Main Entrance
8:45-9:00		Welcome	
9:00-10:30	Marie-Therese Hübsch	Introduction to ab-initio simulations with VASP (DFT, PAW, basic input)	Amphi B
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)	Room P&M Curie
14:30-18:00	(30 min break)	Exercises I: Atoms, molecules and simple bulk	Rooms CP1&2
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	Amphi B
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)	Room P&M Curie
14:30-18:00	(30 min break)	Exercises II: MD and MLFF	Rooms CP1&2
Day III: Wednesday, July 2			
9:00-10:30	Xavier Rocquefelte	The spin degrees of freedom (collinear magnetism)	Amphi B
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)	Room P&M Curie
14:30-18:00	(30 min break)	Exercises III: Magnetism	Rooms CP1&2
19:30		Gala dinner	
Day IV: Thursday, July 3			
9:00-10:30	Manuel Engel	Harmonic and anharmonic phonons	Amphi B
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)	Room P&M Curie
14:30-18:00	(30 min break)	Exercises IV: Phonons and electron-phonon coupling	Rooms CP1&2
Day V: Friday, July 4			
9:00-9:45	Fabien Tran	Exchange-correlation effects revisited (MGGA, hybrids, HF, MBPT)	Amphi B
9:45-10:30	Manuel Engel	Running VASP efficiently	
10:30-11:00		Coffee break	
11:00-12:30		Exercises V: Hybrid functionals	Rooms CP1&2
12:30-14:30		Lunch (Marie Curie - ENSCR)	Room P&M Curie
14:30-...		Round table (feedback)	Amphi B
		Closing	