TYC Materials Modelling Course

Term 1

October 3: Basic many-electron theory: Intro + H atom + He atom +– 2 hours ALS

October 10, October 17: Basic DFT: BA approximation + HF – Thomas-Fermi – Hohenberg-Kohn – LDA – GGA – 4 hours Dave Bowler

October 24, October 31: Periodic boundary conditions – pseudopotentials - electrostatics in DFT – Total energy calculations – Defect formation energies – Charge corrections - 4 hours Tom Durrant

November 7: DFT practicalities and O(N) methods – 2 h Dave Bowler

November 14, November 21: Molecular Dynamics: MD – ab initio MD – time stepping algorithms, classical MD, BO MD, thermostats - 4 hours Jochen Blumberger

November 28; December 5, December 12: Ensembles + KMC: - enhanced sampling - 6 hours (Michail, Alberto)

Term 2

January 9: Kinetics and thermodynamics of nucleation - 2 hours Ian Ford

January 16: Relation between classical forcefields and intermolecular interactions – 2 hours Alberto Striolo

January 23: Interatomic potentials for classical molecular dynamics and Monte Carlo simulations – 2 hours Dorothy Duffy

January 30: Fitting forcefields – 2 h David Gao

February 6, February 13: Phonons – 4 hours Lev Kantorovich

February 20, February 27: Electronic excitations – GW – TDDFT – GF – 4 hours Johannes Lischner

March 6: Accurate ab initio simulations of condensed phases and surfaces– 2 hours Angelos Michaelides

March 13: Quantum MC – 2 hours Dario Alfe

March 20: High throughput computation and structure prediction – 2 hours Chris Pickard