GRADnet SEPnet Modelling Workshop 2015

Old Thorns Manor Hotel, Longmoor Rd, Griggs Green, Liphook, Hampshire GU30 7PE
Sunday 13th December 2015 – Tuesday 15th December 2015

Timetable

Sunday 13th December

1730 – 1830   Guest speaker – materials simulation
1830 – 1900   Dinner

Monday 14th December

Day 1 is devoted to first-principles quantum mechanical simulation of electrons and nuclei. The focus is on the package CASTEP, a full-featured materials modelling code using a plane-wave basis set and pseudopotentials.

0900 – 1000   First-principles materials simulation   Keith Refson
1000 – 1100   Introduction to plane waves and pseudopotentials
1100 – 1130   Refreshments
1130 – 1230   Using CASTEP – the practicalities

1230 – 1400   Lunch

1400 – 1530   Workshop 1 – using CASTEP   Keith Refson
1530 – 1600   Refreshments
1600 – 1700   Workshop 2 - using CASTEP

1730 – 1830   Guest speaker – application of modelling methods in industry

Tuesday 15th December

Day 2 is devoted to molecular dynamics (MD) and Monte Carlo (MC) simulation methods. Students will have the opportunity to tackle one or more simple MC simulation problems in the morning workshop and be introduced to the MD package DLPOLY in the afternoon.

0900 – 1030   Introduction to Monte Carlo methods   David Faux
1030 – 1100   Refreshments
1100 – 1230   Workshop 3 (MC)

1230 – 1400   Lunch

1400 – 1500   Introduction to Molecular Dynamics   Kostya Trachenko
1500 – 1530   Refreshments
1530 – 1700   Using DLPOLY – the practicalities and real examples