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| Session title: | | Applied Monte Carlo: Zeolite Adsorption | | | Course: MC2001 |
| Aims: | | Apply the concepts of Monte Carlo to a real-world example  Demonstrate the full procedure of simulating realistic physical systems using DLMONTE | | | |
| Intended learning outcomes (ILOs) : | | | 1. Describe the use of Monte Carlo methods in current research 2. Demonstrate the use of DLMONTE in simulating realistic systems 3. Interpret the outputs from the Monte Carlo simulation 4. Compare the results of the simulation with those from experiment 5. Change the simulation parameters to better match experimental findings | | |
| Assumed knowledge? | | | From previous sessions:  Basic Monte Carlo theory and methodology, ensembles and use of DLMONTE program.  Adsorption mechanisms | | |
| Timings /min | ILO | | Teacher activity | Learner activity | Resources |
| 0-15 | 1 | | Lecture on background of gases adsorbing to zeolite surfaces. | Listen. | Powerpoint slides:   * Articulate the problem in current research and the usefulness of Monte Carlo techniques * Recap zeolites and adsorption * Examples of standard experimental results |
| 15-120 | 2, 3, 4, 5 | | Provide guidance on exercises, either on an individual or group basis as appropriate. | Work through the practical exercises (based on tutorial 4 of workshop). | Self-contained tutorial based on the adsorption of methane onto a zeolite, either as a Jupyter notebook or a pdf/html document. Will need input files and scripts. Simple answer sheet/guide for demonstrators. |