

**Introduction to Computational Materials Science and Engineering Tools
Short Course**

July 11-12, 2013 • Salt Lake Marriott Downtown at City Creek • Salt Lake City, Utah

Course Schedule:

Thursday, July 11

Density Functional Theory

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| 1:00 - 2:20 p.m. | Introductory Lecture on Density Functional Theory |
| 2:20 - 2:30 p.m. | Break |
| 2:30 - 3:00 p.m. | NanoHUB Account Creation/Introduction to Quantum Espresso |
| 3:00 - 5:00 p.m. | Work on DFT Module Sample Problems |
| 5:00 - 6:00 p.m. | Dinner Break |

Computational Kinetics /Diffusion

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| 6:00 - 7:00 p.m. | Lecture on Computational Kinetics/Diffusion |
| 7:00 - 7:10 p.m. | Break |
| 7:10 - 7:30 p.m. | Walk-through of FiPy on NanoHUB |
| 7:30 - 8:30 p.m. | Work on Kinetics Module Sample Problems |

Friday, July 12

Thermo-Calc

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| 8:30 - 9:30 a.m. | Introductory Lecture on Thermo-Calc |
| 9:30 - 10:00 a.m. | Installation/Break |
| 10:00 - 10:30 a.m. | Lecture on Module Background |
| 10:30 - 11:00 a.m. | Walk-through of Thermo-Calc Examples |
| 11:00 a.m. - 12:00 p.m. | Work on Thermo-Calc Module Sample Problems |
| 12:00 - 1:00 p.m. | Lunch |

Computational Mechanics

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| 1:00 - 2:00 p.m. | Introductory Lecture on Computational Mechanics |
| 2:00 - 2:10 p.m. | Break |
| 2:10 - 4:00 p.m. | Walkthrough of OOF2 |
| 4:00 - 4:10 p.m. | Break |
| 4:10 - 6:00 p.m. | Work on Computational Mechanics Sample Problems |