# Microscale modeling of heat storage materials

**Subject area:** Mechanical Engineering

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| **University:** | TU/e |
| **Level:** | MA all years |
| **Teaching mode:** | completely online, not time-specific |
| **Instructor(s):** | Dr. ir. A.J.H. Frijns |

## Short description

The aim of the course is to present the main approaches for modelling at nano- and microscale level (Density Functional Theory, Molecular Dynamics, Monte Carlo) in order to facilitate the computation and the understanding of the heat and mass transfer phenomena on small scales and to apply the knowledge to heat storage materials.

## Full description

For designing heat storage materials and devices, a good physical understanding of the phenomena is needed and proper (numerical) models are required. On the nano- and microscales the local properties cannot be averaged out anymore and individual particle properties have to be taken into account, boundary effects and surface and interface forces become dominant.
In this course we will start at the basis: the interactions that take place at the atomic and molecular level. We will show that these small interactions sometimes can have major influences on macroscopic level, e.g. structures stability, reactivity, slip velocities and temperature jumps. We start modelling at the atomic/molecular level (Density Functional Theory simulations followed by Molecular Dynamics models for heat and mass transfer) and scale it up via Monte Carlo models (MC). We will show that by using the appropriate assumptions these models can be directly connected to each other.
The characteristic properties described on molecular level are used to understand the transport, thermal and kinetic properties of heat storage materials and interface properties in micro/nano systems.

## Learning outcomes

After passing the course, the student is able to:

- Understand the structure of matter and explain the main experimental techniques for structure determination;
- Understand the concepts of molecular dynamics (MD), including intermolecular interactions, and knows how to derive macroscopic properties from molecular positions and velocities;
- Model fluid-solid interactions, including reflective, diffusive and explicit walls;

- Understand the concepts of Direct Simulation Monte Carlo (DSMC) methods, understand the similarities and differences with MD;
- Model adsorption in porous media for energy storage;
- Understand the Density Functional Theory (DFT), Chemical Bonding analysis and Machine learning;
- Apply above theories for porous media and micro/nanochannel devices.

## General information

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| **Contact hours per week:** | Q&A sessions |
| **Total workload:** | 140 (in student hours for the whole course) |
| **ECTS credits:** | 5 |
| **Language:** | English |
| **Course start date:** | 14 November 2022 |
| **Course end date:** | 20 January 2023 |
| **Add. info about start date:** | |
| **Weekly teaching day/time:** | |
| **Time zone:** | CET (Denmark, Germany, France, Netherlands, Switzerland, Czech Republic) |
| **Further information:** | e-learning (online knowledge clips, quizzes, short assignments, direct feedback) & weekly Q&A sessions (via Teams, exact time slot will be announced later) |
| **Prerequisites:** | Understanding of and basic knowledge on:<br>• definitions and basic concepts of thermodynamics (equations of state, state variables, systems, processes, ideal gas law)<br>• conductive, convective, and radiant heat transfer and non-dimensional numbers<br>• partial differential equations (PDEs)<br>• basic programming skills in Matlab or Python |
| **Activities and methods:** | Tutorial sessions |
| **Presence on campus:** | |

## Final examination

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| **Form:** | written |
| **Date:** | |
| **Location/format:** | online |
| **Re-sit possibility:** | yes |
| **Transcript available:** | end of semester |
| **Add. info/requirements:** | |

## Registration

To register for this course, follow the registration requirements of your **home university** as specified here: www.euroteq.eu/courses-registration.

## Administration

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| **Number of places:** | 20 |
| **Minimum participants:** | |
| **Internal course code:** | 4SE20ONL |
| **Contact:** | A.J.H.Frijns@tue.nl |

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*This course is part of the EuroTeQ Engineering University joint course catalogue 2022/2023. This is a collaborative activity of the partner universities DTU, L'X, TU/e, TalTech, CTU, TUM as well as Technion. Students from these universities can participate in the offered courses. It is the responsibility of the student to check if you fulfil the requirements to participate in a specific course. Students are also advised to check with their home institution how to get recognition of the ECTS credits gained in courses of the EuroTeQ course catalogue. For further information about EuroTeQ Engineering University, visit www.euroteq.eu or get in touch with the above-mentioned point of contact.*