

## MM 21: Materials for Storage and Conversion of Energy: Energy Conversion

Time: Tuesday 14:15–15:30

Location: SCH A 215

MM 21.1 Tue 14:15 SCH A 215

**Harvesting of low-grade waste heat with shape memory alloys** — ●BRUNO NEUMANN<sup>1,2</sup> and SEBASTIAN FÄHLER<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf — <sup>2</sup>Technische Universität Dresden

More than half of all energy converted by humankind is lost in the form of waste heat. Not only does that strongly contribute to the acceleration of global warming, it also leaves an enormous economic potential untouched. However, suitable technologies are limited, since most of this heat is of low temperature ( $< 100$  °C). In the last years, materials and technologies for thermoelectric harvesting and thermomagnetic harvesting have been explored, but a high efficiency of those systems remain a challenge. With our work, we present a thermoelastic harvesting approach for converting the waste heat of a fluid into electricity, utilizing shape memory alloy wires. These wires bring the inherent advantage that their transformation temperatures can be adapted to the required temperature range of the waste heat. Moreover, they provide a very high actuation energy density and are commercially available. In our set-up, we use two mechanically connected arrays of wires to reach a high power density of the system. Our simulation data predicts a thermodynamic efficiency in respect to the Carnot efficiency of 22.7 %, which exceeds current efficiency benchmarks set by thermoelectric materials.

MM 21.2 Tue 14:30 SCH A 215

**Atomistic simulations of the Seebeck effect in electrolytes** — ●OLE NICKEL<sup>1</sup>, MATHIJS JANSSEN<sup>2</sup>, and ROBERT MEISSNER<sup>1</sup> — <sup>1</sup>Hamburg University of Technology, Hamburg, Germany — <sup>2</sup>University of Oslo, Oslo, Norway

The Seebeck effect allows electrical energy to be obtained directly from thermal gradients. In electrolytes it is based on an differential heat of transport of the ions.

We perform molecular dynamic simulations with different electrolytes between graphene electrodes. We apply an external resistance between the electrodes via a thermopotentiostat, where the thermal fluctuation term is deactivated, effectively resembling an RC-circuit with a time constant of  $\tau=RC$ .

With this method it is possible to simulate a complete electrochemical cell in open circuit conditions which is charged with a thermal gradient and then discharged at constant temperature. The Seebeck energy is the energy that is dissipated across the external resistance. The goal is to investigate optimal electrolyte parameters to maximize this energy.

MM 21.3 Tue 14:45 SCH A 215

**Non-Local DFT calculations towards the discovery of stable water-splitting catalysts** — ●AKHIL S. NAIR, LUCAS FOPPA, EVGENY MOERMAN, and MATTHIAS SCHEFFLER — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin, Germany

Efficient prediction of the thermodynamic and aqueous stability of materials is essential for leveraging the catalyst discovery for the water splitting reaction. In particular, the oxygen evolution half-reaction is

usually carried out using oxide catalysts under harsh potential and pH conditions.[1] This necessitates the application of DFT methods which can predict the oxide stability under experimentally relevant conditions without any *ad hoc* corrections.[2] In this regard, herein, we employ a non-local DFT method using the hybrid HSE functional for calculating the stability of oxide catalysts. Crucially, we scrutinize the effect of the HSE mixing parameter on the formation energies and aqueous stability of oxides and compare to higher-level calculations using coupled-cluster theory for reference systems. Through this approach, we attempt to standardize the application of HSE method for accurate oxide stability prediction which could augment the large-scale catalyst discovery.

[1] Z.Wang, *et al.*, *npj Comput. Mater.* **6**, 160 (2020).

[2] L.-F. Huang, J. M. Rondinelli, *npj Mater. Degrad.* **3**, 26 (2019).

MM 21.4 Tue 15:00 SCH A 215

**Photocatalytic water splitting from Koopmans spectral functionals: The case of  $TiO_2$  polymorphs** — ●MARIJA STOJKOVIC<sup>1</sup>, EDWARD LINSKOTT<sup>1</sup>, and NICOLA MARZARI<sup>1,2</sup> — <sup>1</sup>Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — <sup>2</sup>Laboratory for Materials Simulations, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Photocatalytic water splitting has drawn considerable attention for renewable energy production. Since the first reported photocatalytic water splitting by titanium dioxide, this material remains one of the most promising photocatalysts, due to its suitable band gap and band-edge positions. However, estimating both of these properties is a challenging task for standard DFT functionals. Here we show how Koopmans spectral functionals can accurately predict the band structure and level alignment of rutile, anatase and brookite, demonstrating the advantage of orbital-density dependent functionals for predicting the spectral properties of materials.

MM 21.5 Tue 15:15 SCH A 215

**DFTB Description of the Ground and Excited States Properties of Thiolate Protected Gold Nanoclusters** — ●CARLOS R. LIEN-MEDRANO<sup>1</sup>, ARNAUD FIHEY<sup>2</sup>, and THOMAS FRAUENHEIM<sup>1</sup> — <sup>1</sup>University of Bremen, Bremen, Germany — <sup>2</sup>University of Rennes, Rennes, France

Gold nanoclusters stand as promising building blocks for solar energy harvesting applications, luminescent materials and catalytic devices. At the frontier between molecular and metallic structures, their large number of electrons prevent the use of *ab initio* quantum mechanic method to rationalize and predict their structure-property relationships, especially when fully coated with organic ligands. Using a semi-empirical DFT-based scheme, namely Tight-Binding Density Functional (DFTB), we demonstrate that it is possible to rapidly access the ground (geometry and electronic structure) and excited state (UV-Visible absorption) properties of these nano-objects without sacrificing the qualitative accuracy of its parent DFT, paving the way towards a quantum material design of gold-organic nano-devices.