MM 16: Functional Materials II

Time: Tuesday 14:00–15:45 Location: SCH/A216

MM 16.1 Tue 14:00 SCH/A216

Low and High Dose Gamma Radiation Effect on Germanium-Doped Optical Fibers: Investigation of Color Centers — •Esra Kendir Tekgül — Bilkent University UNAM, Institute of Materials Science and Nanotechnology, Ankara, 06800, TURKEY

Ge-doped optical fibers are widely used in sensing, data transmission, and space technologies, making their radiation resistance crucial. Gamma irradiation creates radiation-induced defects that form color centers, degrading optical transmission. In this study, five Ge-doped fibers and one quartz fiber were exposed to gamma rays of 0.5-50 kGy. RIA values at 550, 600, 680, and 755 nm were measured before and after irradiation, and color centers were identified from the RIA spectra. GeX, Ge-NBOHC, and GeY defects were attributed to Ge contributions, whereas ODC(II), STH1, and STH2 were attributed to the SiO2 matrix. NA and FTIR results showed radiation-induced changes in refractive index and a decrease in NA. Overall, the findings highlight the potential of Ge-doped fibers for radiation-hard applications and dosimetric sensing.

MM 16.2 Tue 14:15 SCH/A216

Switching applications in optical circuits using the electrochromic properties of LiMn2O4 — •Vinit Kumar Agarwalla[1], Yug Joshi[2], Guido Schmitz[1], and Mayank Kedia[3] — [1]Institut für Materialwissenschaft, Universität Stuttgart, Stuttgart Germany — [2]Max Planck Institute for Sustainable Materials, Dusseldorf, Stuttgart — [3]Institut für Photovoltaik, Universität Stuttgart, Stuttgart Germany

Optical communication depends on the accuracy with which the path of light is controlled to minimize signal loss in waveguides. The current method of optimizing the path of light is to maintain the waveguide's refractive index using the thermooptic effect. The waveguide consists of a core in which light travels, surrounded by cladding material to ensure total internal reflection, and a third protective outer layer. Here, I propose using electrochromic lithium manganese oxide(LiMn*O*, LMO) as a waveguide cladding. The primary wave from the core extends into the cladding known as evanescent waves, so changing the cladding*s refractive index changes the evanescent waves' path and thus the entire path of the light. Previous work has shown a change in refractive index in the visible region. Building on that, we measured IR reflectance spectra showing continuous visible-to-IR transitions, 100% reflectance, and resonance shifts with lithiation. Calculations show that a 38 μm waveguide can induce a π phase shift at 1550 nm. We also propose various delithiation methods to alter optical properties without degrading the optical structure.

MM 16.3 Tue 14:30 SCH/A216

In-Situ Activation of a Monolithic SrTiO3 Single Crystal for Room Temperature Hydrogen Sensing — •Karl-Michael Weitzel, Timo Kassubek, and Kevin Rein — Department of Chemistry, Philipps-Universität Marburg, Marburg, Germany

The development of reliable, fast, and cost-effective hydrogen sensors is of increasing importance for the safe implementation of a hydrogen-based economy. This work presents a novel and simple single-step method to convert an insulating strontium titanate (SrTiO3) single crystal into a highly sensitive, monolithic hydrogen sensor that operates at room temperature. The activation is achieved by applying a moderate DC electric field (100 V/cm) across a symmetric Pt/SrTiO3/Pt capacitor structure at 180 °C in a pure hydrogen atmosphere (200 mbar). This process causes a drastic and stable reduction in the material's resistance by several orders of magnitude. We propose a model of "field-induced chemical doping" to explain this transformation. The resulting activated crystal exhibits excellent hydrogen sensing properties at room temperature, detecting molecular hydrogen (H2) over an exceptionally wide partial pressure range from 0.0001 mbar to 1000 mbar with an accuracy of a few percent. The sensing mechanism is based on the reaction of hydrogen with the activated SrTiO3 sample, involving the release of electrons back into the conduction band and lowering the device's resistance. This monolithic approach opens a new pathway for designing robust and easy-to-fabricate chemical sensors from wide-bandgap oxides.

MM 16.4 Tue 14:45 SCH/A216

The laser-induced synthesis of Co-MOFs, the investigation of optic, gase sorption, DFT and sensor properties — Saliha MUTLU[1,2], Bülend ORTAÇ[2], Ali KARATUTLU[2,3], Taylan GÖRKAN[2], Engin DURGUN[2], Dilek SÖYLER[4], Saniye SÖYLEMEZ[4], Jelena LILLEPÄG[5], Volkan FILIZ[5], Nergis ARSU[6], and •Sevil SAVAŞKAN YILMAZ[1] — [1]Karadeniz Technical University Chemistry Department, Trabzon, Türkiye — [2]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [3]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [4]Department of Biomedical Engineering, Necmettin Erbakan University, Konya, 42090 Turkey — [5]Helmholtz-Zentrum Geesthacht, Institute of Polymer Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany — [6]Yildiz Technical University, Department of Chemistry, Davutpasa Campus, Istanbul, 34220 Turkey

High-power rapid laser-induced synthesis of MOFs has drawn significant attention due to the rapid and effective preparation conditions for Zn- and Ni-MOFs. In this study, the Co-MOF microcrystals yield visible light photoluminescence with relaxation times on the order of ns, showing controllable properties, including low-temperature paramagnetic state transition, supported by magnetic measurements and DFT calculations. Outstanding performance in gas sorption and electrochemical sensing has been demonstrated with low separation costs and ultra-low LODs for dopamine, respectively.

MM 16.5 Tue 15:00 SCH/A216

First-Principles Study of Electronic and Optical Properties of Mo-Doped $CsPbBr_3$ Perovskites — Said Al Azar[1], Anas Al-Reyahi[2], •Saleh Bashaish[3], and Marwan Mousa[4] — [1]Zarqa University, Zarqa, Jordan — [2]Hashemite University, Zarqa, Jordan — [3]Al-Ahliyya Amman University, Amman, Jordan — [4]Jadara University, Irbid, Jordan

$CsPbBr_3$ perovskites, particularly when doped, show great promise for tandem solar cells and advanced optoelectronics. This study employs density functional theory (DFT) and semi-classical Boltzmann transport theory to comprehensively investigate the structural, electronic, magnetic, thermoelectric, and optical properties of Mo-doped $CsPb_{(1-x)}Mo_xBr_3$ (x = 0, 0.25, 0.5, 0.75). Our calculations confirm the structural stability of all compositions and reveal a transformative electronic behavior: Mo-doping induces a ferromagnetic half-metallic state. Notably, the $x = 0.5$ composition exhibits an ideal band gap for solar applications (1.872 eV via mBJ) and a high spin-up figure of merit (zT) approaching unity at room temperature. Additionally, enhanced absorption in the infrared region suggests potential for IR photodetectors. These findings establish Mo-doped $CsPbBr_3$ as a compelling multifunctional material for spintronic and high-efficiency optoelectronic devices.

MM 16.6 Tue 15:15 SCH/A216

Optimizing NiTi Interatomic Potentials Through Atomic Cluster Expansion — •Petr Šesták[1,2], Petr Jaroš[1], Miroslav Černý[2], and Petr Sedlák[1] — [1]Institute of Thermomechanics Czech Academy of Sciences, Prague, Czechia — [2]CEITEC, Brno University of Technology, Brno, Czechia

In this work, we present an interatomic potential for NiTi based on the Atomic Cluster Expansion, developed using the Pacemaker software package. We validate this potential by comparing it against the results of simulations using other interatomic potentials, quantum-mechanical calculations, as well as our own experimental data. Our quantum-mechanical calculations utilize density functional theory (DFT) within the generalized gradient approximation (GGA) to determine the ground-state structural, electronic, thermodynamic, and elastic properties of NiTi in low-temperature (martensitic) phase. The target properties include elastic constants, phonon spectra calculations, and vacancy formation energy. Specifically, the stress-strain method was employed to compute the full tensor of the second-order elastic constants and assess the mechanical stability of the studied phases, ensuring that the results are consistent with those obtained using other established potentials.

MM 16.7 Tue 15:30 SCH/A216

Response of NiTi martensite to mechanical loading — •Miroslav Černý and Petr Šesták — Central European Institute of Technology, CEITEC, Brno University of Technology, Purkyňova 123, Brno, Czechia

Shape-memory alloys are unique materials capable of undergoing large reversible strains and exhibiting the shape-memory effect, which is driven by external changes of temperature. These remarkable properties are based on a martensitic transformation between austenite (high-temperature phase) and martensite (low-temperature phase). The NiTi shape memory alloy has become the most widely used shape memory material in industrial, high-tech, and medical ap-plications due to its unique thermal and mechanical properties.

In this work we aim at fundamental understanding of the behavior of twins in the martensite structure under mechanical loading. For this purpose, we constructed computational supercells representing both the perfect and twinned martensite and studied their responses to shear and tensile loading. Such calculations are computationally very demanding when using ab initio approaches. Therefore, we employed machine learning to develop a new interatomic potential, tailored specifically for the martensite struc-ture. Computationally accessible predictions based on the potential were benchmarked from first principles.