**Scientific Program**

**“Recent Advances in Computational Modeling for Energy Applications”, Tuesday, July 7 2015**

**David Wang Auditorium, 3rd floor of Dalia Meidan Building at the Materials Science & Engineering Department, Technion, Haifa**

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| 8:00-9:00 | Gathering and registration |
| 9:00-9:05 | Maytal Caspary Toroker, Technion, opening remarks |
| Session 1 | Chair: Oswaldo Dieguez, TAU |
| 9:05-9:30 | Dan Mordehai, Technion, “Mechanical Properties of Crystalline Nanoparticles”  |
| 9:30-9:55 | Nino Russo, Università della Calabria, “H2 production in homogenous phase” |
| 9:55-10:20 | Irena Efremenko, Weizmann, “Computational exploration of polyoxometalates" |
| 10:20-11:00 | Break |
| Session 2 | Chair: Ana Muñoz Garcia, University of Naples Federico II |
| 11:00-11:25 | Leeor Kronik, Weizmann, “Multiscale approach to the electronic structure of doped semiconductor surfaces” |
| 11:25-11:50 | Michele Pavone, University of Naples Federico II, “Ab initio simulation of p-type dye-sensitized solar cells: effects of different anchoring groups on dye-electrode interfacial properties” |
| 11:50-12:15 | Oded Hod, TAU, “Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index” |
| 12:15-14:00 | Lunch+poster session |
| Session 3 | Chair: Arik Yochelis, BGU |
| 14:00-14:25 |

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| Guy Makov, BGU, "Ab-initio prediction of thermophysical properties in metals: Ti and Zr as a case study" |

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| 14:25-14:50 | Noa Marom, Tulane University, “Toward Computational Design of Cluster-Based Functional Nano-Structures“ |
| 14:50-15:15 | Oswaldo Dieguez, TAU, “Bismuth manganite films: larger polarization and smaller band gap than typical perovskite oxides” |
| 15:15-15:45 | Break |
| Session 4 | Chair: Guy Makov, BGU |
| 14:45-15:10 | Dan T. Major, BIU, “First principles modeling of battery materials“ |
| 15:10-15:35 | Amir Natan, TAU, “Affordable Hartree-Fock in real-space using projector operators**”** |
| 15:35-16:00 | Arik Yochelis, BGU, “Why dynamical systems approach is essential to our understanding of electrochemical aspects of ionic liquids” |
| 16:00-16:25 | Joan Adler, Technion, “Visualization of electronic density from Quantum Espresso calculations” |
| 16:25-16:30 | Maytal Caspary Toroker, Technion, closing remarks |