**Poster List**

**“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**

1. “Thermodynamic properties of titanium from ab initio calculations”

Uri Argaman , Eitan Eidelstein, Ohad Levy and Guy Makov

1. “Visualization of Electronic Density of Nanotube with AViz”

Omri Adler, Joan Adler, Bastien Grosso, Polina Pine, Yuval Yaish

1. "Graphitization in Irradiated Diamonds using Molecular Dynamics"

Omri Harosh, Joan Adler, Rafi Kalish, Amihai Silverman

1. “AViz – Atomistic Visualization”

Jeremy Rutman, Amihai Silverman, Joan Adler, Adham Hashibon, Nathan Franklin

1. “Electronic properties of nanometric semiconductors from *ab initio* calculations”

Elad Segev, Guy Makov

1. “Frequency and Zero-Point Vibrational Energy Scale Factors for Double-Hybrid Density Functionals (and Selected Other Methods): Can Anharmonic Force Fields Be Avoided?”

Manoj K. Kesharwani, Brina Brauer, and Jan M.L. Martin

1. “Molecular Dynamics Simulations of Dislocation Dynamics”

Eyal Oren, Guy Makov

1. “New Benchmark Study on C20 and C24 Isomers”

Debashree Manna, Jan M. L. Martin

1. “The Pt/alpha-Fe2O3 interface”

Ofer Neufeld, Maytal Caspary Toroker

1. “Electronic structure of pure, doped and alloyed Fe2O3:Nb2O5: an ab initio study”

Natav Yatom, Maytal Caspary Toroker

1. “Oxyhydroxides of transition metals catalysts for electrochemical water splitting”,

Jeremie Zaffran, Maytal Caspary Toroker

1. “Electronic structure of Fe-Ni oxyhydroxide”,

Valeria Butera, Vicki Fidelsky, Jeremie Zaffran, Maytal Caspary Toroker.

1. “Efficient integral method for electrostatic potentials within the PARSEC real-space code”

Michal Zuzovski, Amir Boag, Amir Natan

1. “Diffusion of O2 in PFC and TEGDME: A molecular dynamics study”

Natalia Kuritz, Michael Murat, Moran Balaish, Yair Ein-Eli, Amir Natan

1. “Classical and quantum modeling of Li and Na diffusion in FePO4”

Mudit Dixit, Hamutal Engel, Reuven Eitan, Doron Aurbach, Mikhael D. Levi, Monica Kosa, Dan Thomas Major

1. “Comparative Study of the electronic structure of Co-based mixed and single valence compounds: search for efficient PV materials”

Vijay Singh, Monica Kosa, Koushik Majhi, Dan Thomas Major