The quest for descriptors in high-throughput searches: thermoelectrics and topological insulators

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High-throughput computational materials design is an emerging area of materials science [1]. By combining advanced thermodynamic and electronic-structure methods with intelligent data mining and database construction, and exploiting the power of current supercomputer architectures, scientists generate, manage and analyze enormous data repositories for the discovery of novel materials [2].
The key for discovering new materials is the availability of descriptors. These are physically sound empirical quantities, not necessarily observables, connecting the calculated microscopic parameters to macroscopic properties of the materials. In other words, the descriptor is the language with which the researcher speaks to the database, the heart of any effective HT implementation.
In this talk **(i)** we provide a current snapshot of this rapidly evolving field (e.g. catalysis [3], thermodynamics [4], battery materials [5], thermoelectricity [6,7], topological insulators [8], photovoltaics [9], water splitting [10,11], nuclear detection [12], nuclear detection, and so on), **(ii)** we highlight the challenges and opportunities that lie ahead, and **(iii)** we illustrate the needs and goals of the communities involved: open and free repositories with widely accepted standards [13].

[1] Nature Mater, **12**, 191 (2013). [2] http://aflowlib.org - http://materialsproject.org [3] Nature Mater. **5**, 909 (2006). [4] Comp. Mat. Sci. **58**, 227 (2012). [5] Mater. Res. Soc. Bull. **35**, 693 (2010). [6] Phys. Rev. X **1**, 021012 (2011). [7] Carrete, Li, Mingo, Wang, Curtarolo, "*Finding unprecedentedly low thermal conductivity compounds via HT materials modeling*", (2013). [8] Nature Materials **11**(7), 614 (2012). [9] Phys. Rev. Lett. **108**, 068701 (2012). [10] Energy Environ. Sci. **5**, 5814 (2012). [11] Energy Environ. Sci. **6**, 157 (2013). [12] ACS Comb. Sci. **13**, 382 (2011). [13] "*Fuelling discovery by sharing*", Nature Mater. **12**, 173 (2013).