Future Prospects for Data-Driven Methods in Materials Science
Outline

I. OUTLINE

- Framing AM as a sub-field of materials science: other fields have tackled similar problems
  - High-throughput studies have long been used in materials science [**?**]
  - Multi-scale modeling has also been around in materials for a while [1]
  - Machine learning has been adopted in materials recently
  - **AM users do not need to reinvent the wheel (completely) when adopting data-driven methods for AM; they need to look to previous investigations in materials science**
- Data driven/machine learning has been picking up in materials
  - Promoted by materials genome initiative [2]
  - Examples:Photovoltaic materials [**?**]; Dialetric Materials [3]; Molecule Design [4]; [5]
  - Adoption of machine learning in AM should take into consideration how other fields are using it **so that standard applications of ML in materials science can be developed**
  - Review articles of ML for mat sci: [6–9]
  - **The AM field, along with other fields of mat sci, should evolve toward standard practices in the use of machine learning**
  - Maybe a good place to talk about standard data formats (e.g. the PIF)
  - The 'standard' adoption of ML (and what it would look like) is something that Branden, Brice, etc., may have insight on
- Moving AM toward a database-driven approach
  - Other fields are already adopting databases: Mat Proj [10], AFLOW [11]; OQMD
  - **Machine learning models can be improve with more data, therefore AM data should be widely & publicly accessible**
  - Discuss infrastructure necessary for use of AM databases

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[1] in *Proceedings of the 2nd World Congress on Integrated Computational Materials Engineering (ICME)*, edited by M. Li, C. Campbell, K. Thornton, E. Holm, and P. Gumbsch (TMS (The Minerals Metals, and Materials Society), Salt Lake City, UT, 2013).

[2] J. J. De Pablo, B. Jones, C. L. Kovacs, V. Ozolins, and A. P. Ramirez, Current Opinion in Solid State and Materials Science **18**, 99 (2014), arXiv:arXiv:1011.1669v3.

[3] C. Kim, G. Pilania, and R. Ramprasad, Chemistry of Materials **28**, 1304 (2016).

[4] K. T. Butler, D. W. Davies, H. Cartwright, O. Isayev, and A. Walsh, Nature Reviews **559** (2018).

[5] A. Mannodi-Kanakkithodi, G. Pilania, T. D. Huan, T. Lookman, and R. Ramprasad, Nature Scientific Reports **6**, 1 (2016).

[6] R. Ramprasad, R. Batra, G. Pilania, A. Mannodi-Kanakkithodi, and C. Kim, Nature Computational Materials **3** (2017).

[7] S. R. Kalidindi, D. B. Brough, S. Li, A. Cecen, A. L. Blekh, F. Y. P. Congo, and C. Campbell, Materials Research Society Bulletin **41** (2016).

[8] N. Wagner and J. Rondinelli, Frontiers in Materials **3** (2016).

[9] A. Jain, G. Hautier, S. P. Ong, and K. Persson, Materials Research Society **31** (2016).

[10] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, APL Materials **1** (2013), 10.1063/1.4812323.

[11] S. Curtarolo, W. Setyawan, G. L. W. Hart, M. Jahnatek, R. V. Chepulskii, R. H. Taylor, S. Wang, J. Xue, K. Yang, O. Levy, M. J. Mehl, H. T. Stokes, D. O. Demchenko, and D. Morgan, Computational Materials Science **58**, 218 (2012), arXiv:1308.5715.