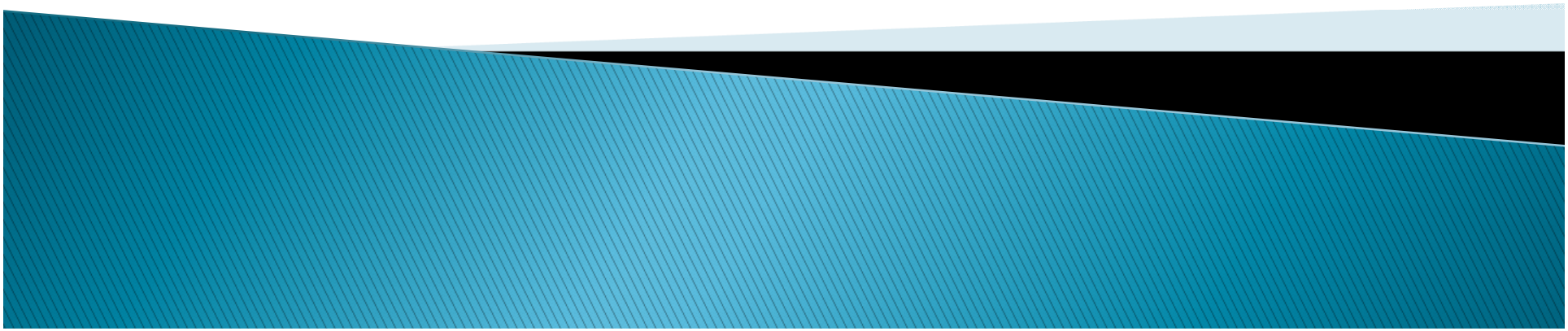
Modelling Across Scale

Stanley M. Howard
Dept of Materials and Metallurgical Engineering
SDSM&T



Dr. Howard

- Before College — Cheyenne, WY
- College — Colorado School of Mines

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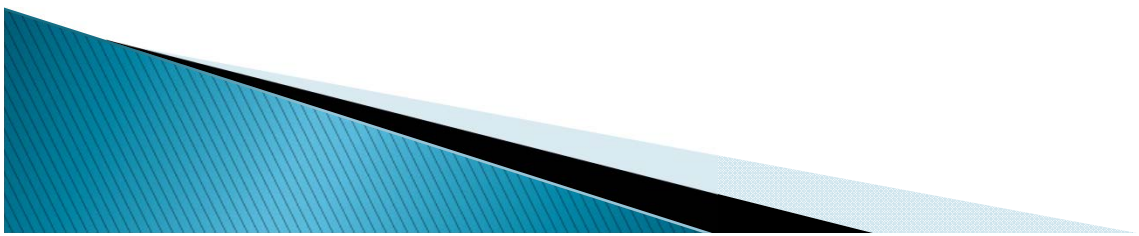


Career History

- 1971 – present SDSM&T Department of Materials and Met Eng
- Assistant Professor (1971 – 75),
- Associate Professor (1975 – 81)
- Professor (1981–2014), Chair (1994–2000)
- Professor Emeritus and Senior Lecturer (2014–present)
- 2016 – 2017 TMS President, Warrendale, PA
- 2004 – 2007 Yucca Mountain Project, Consultant, Summerlin, NV
- 2003 – 2004 Oak Ridge Nat'l Lab, Oak Ridge, TN
- 1992 – 2001 Caterpillar Corporation – Consultant, Peoria, IL
- 1988 – 1991 Electronic Man. Consultant, U. S. Navy, Ridgecrest, CA
- 1986 – 1987 Kerr–McGee Corporation, Consultant, Oklahoma City, OK
- 1981 – 1988 Group V Metals, Inc. – President (1981–4), Rapid City, SD
- 1977 – 1982 Mintech, Inc. – President (1977–82), Rapid City, SD
- 1976 – 1977 Stanford Research Center, NSF Visiting Sci, Menlo Park, CA
- 1967 – 1971 Dept of Metallurgical Eng, Research Fellow, CSM
- 1967 Atomic Weapons Div., Dow Chemical Company, Golden, CO

Thought of the Day

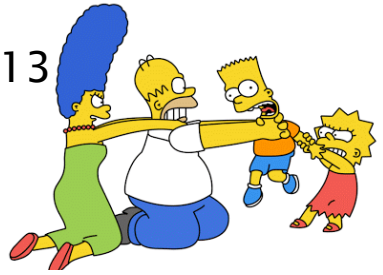
Dealing with insult

- **Anger** This is the weakest possible response
  - It shows that we take the insult and the insulter, seriously.
  - It suggests that there is truth in the insult.
  - It destabilizes us and causes us pain.

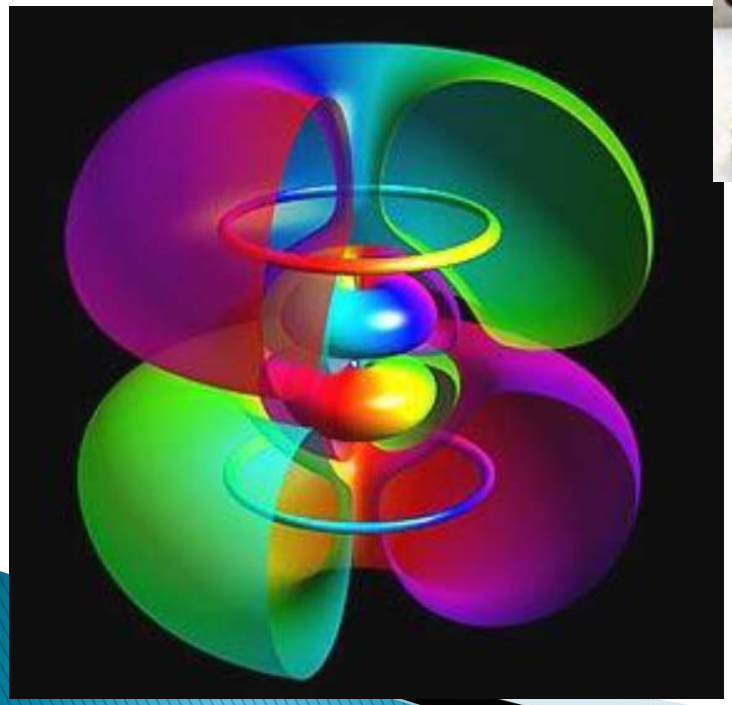
- **Acceptance**. This the strongest response.

  Consider three things:
  - Is the insult true? Who did it come from and why?
  - If the insult is true, the person it came from is your advocate, then the *insult* is more likely a statement of useful fact.

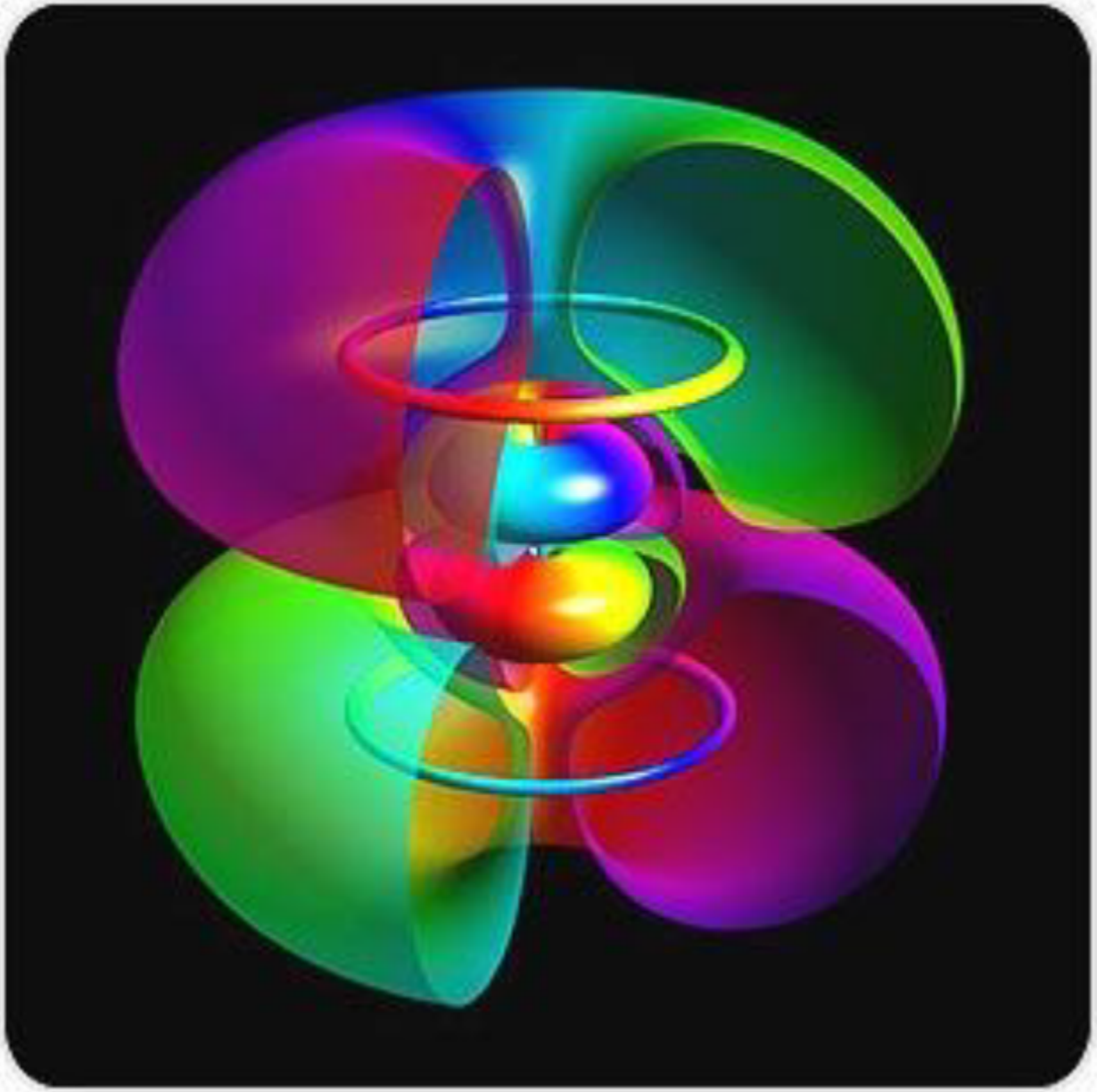
Neel Burton, MD, Psychology Today, Feb 13, 2013



From atomic characteristics to engineering material properties



Wavefunction Approach



Really hard to

$$|\Psi(\vec{r}_1, \vec{r}_2, \ldots)$$

Ea

Why? Because of Hermi

$$O(\vec{r}) = \Psi^\dagger(\vec{r}_1, \vec{r}_2, \ldots)($$

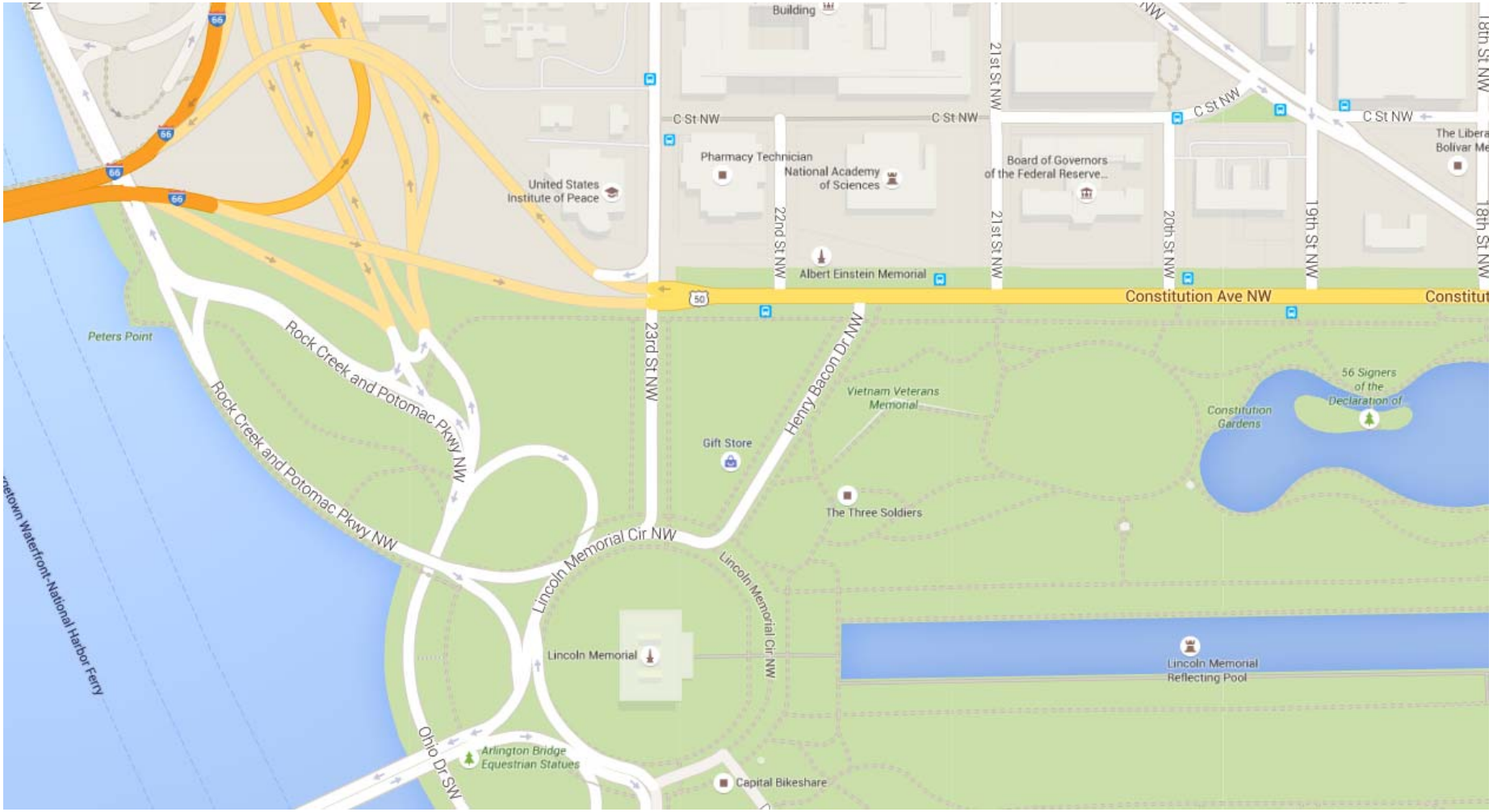
Kinetic Energy Density:

$$\tau(\vec{r}) = \Psi^\dagger(\vec{r}_1, \vec{r}_2, \ldots) \left[-\frac{1}{2} \right.$$

Credit:

PETER W. VOORHEES

Frank C. Engelhart Professor of Materials Science and Engineering
Department of Materials Science and Engineering
MCCORMICK SCHOOL OF ENGINEERING
NORTHWESTERN UNIVERSITY


Building
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United States Institute of Peace
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19th St NW
18th St NW
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Constitution Ave NW
Peters Point
Rock Creek and Potomac Pkwy NW
23rd St NW
Henry Bacon Dr NW
Vietnam Veterans Memorial
56 Signers of the Declaration of
Constitution Gardens
Gift Store
The Three Soldiers
Rock Creek and Potomac Pkwy NW
Lincoln Memorial Cir NW
Lincoln Memorial Cir NW
Lincoln Memorial
Lincoln Memorial Reflecting Pool
Ohio Dr SW
Arlington Bridge Equestrian Statues
Capital Bikeshare

NAE Building in DC

WOLVERTON Research Group

Machine Learning

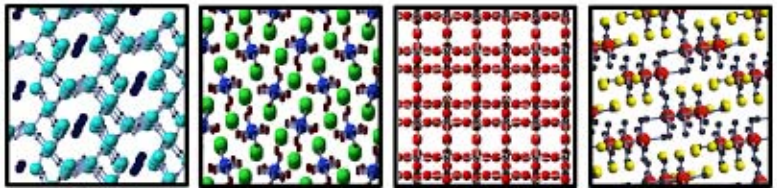
Overview

Machine learning algorithms are designed to automatically extract new knowledge out of data. One focus of the Wolverton group is to use machine learning to learn more about materials and to create models that can be used to discover new materials. In some of our recent work (described below), we have used machine learning to discover new ternary compounds and create useful empirical rules for predicting the solubility of various elements in zirconia. We are currently working to expand the techniques demonstrated in these examples to other materials system and are developing tools to make these capabilities available to the materials science community at large.

Discovering Novel Ternary Compounds

Reference: Meredig, Agrawal *et al.* Physical Review B, 89 (2014), 094104.

Discovering new crystalline compounds is very computationally expensive process and is often approached in two distinct ways. In one method, one selects a single composition or alloy system where experimental results suggest it might be possible to form a new compound and then evaluate up to thousands of possible crystal structures



The Minerals, Metals, and Materials Society

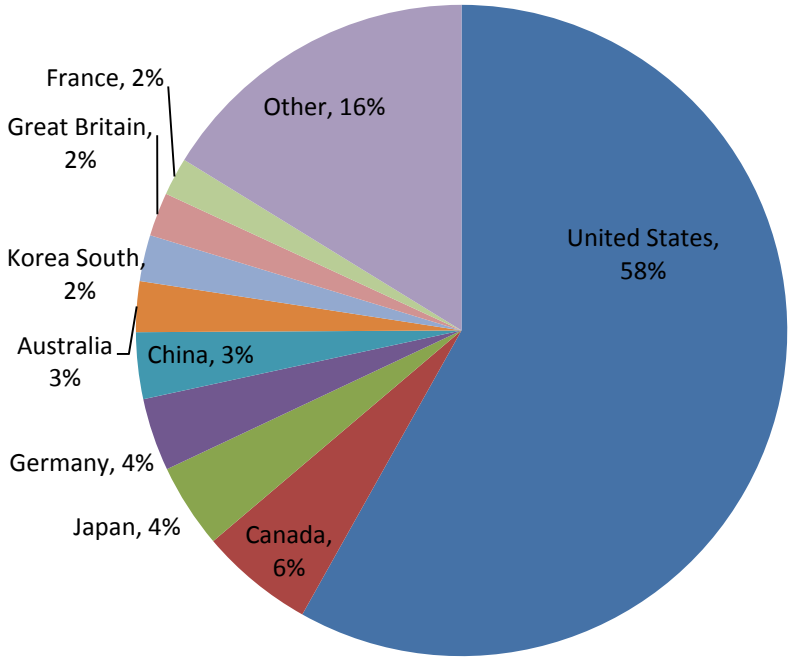
Warrendale, PA, US

2014 Membership Breakdowns

TMS Membership Profile	
Professionals	7,514
Students	5,369
Total	12,883

Professional Member Employers	
Industry	40%
Academia	42%
Government	12%
Retired	4%
Unknown	2%

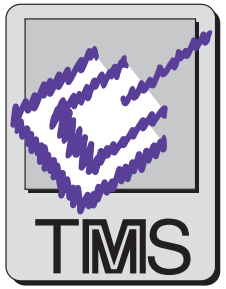
Professional Members Region

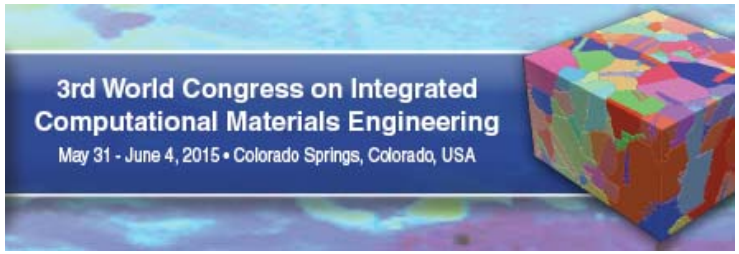


Diversity Awards

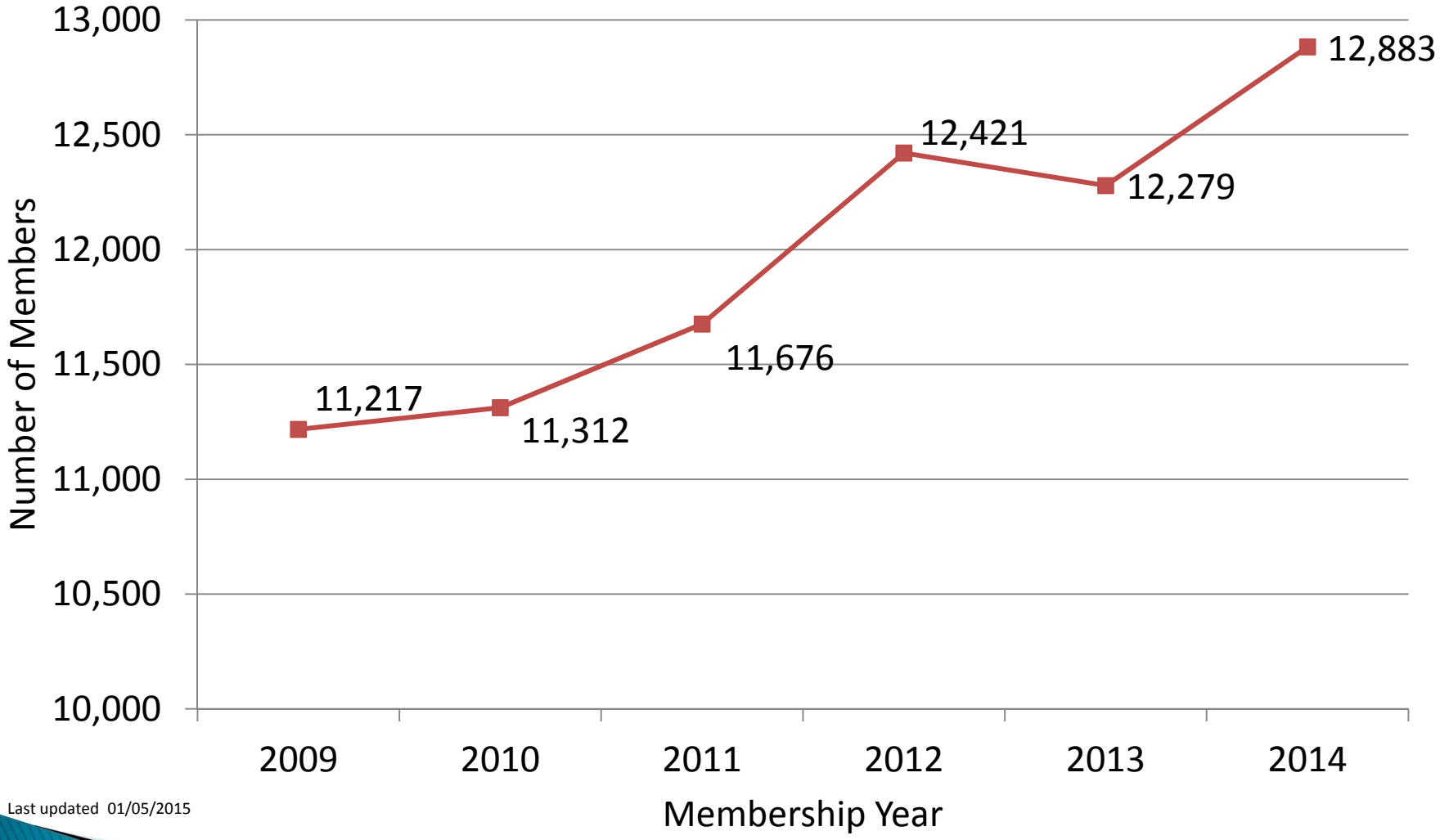
- Ellen Swallow Richards Diversity Award: recognizes a member of the materials community who has helped others overcome diversity challenges. Debut: 2014.
- Frank A. Crossley Diversity Award: recognizes a member of the materials community who has personally overcome diversity challenges. Comes with a $1,500 cash prize. To be first awarded in 2016.
- *Both awards endowed by Battelle CEO Jeff Wadsworth and his wife, Jerre.*

TMS Global Meetings





TMS Membership: 2009–2014



Last updated 01/05/2015

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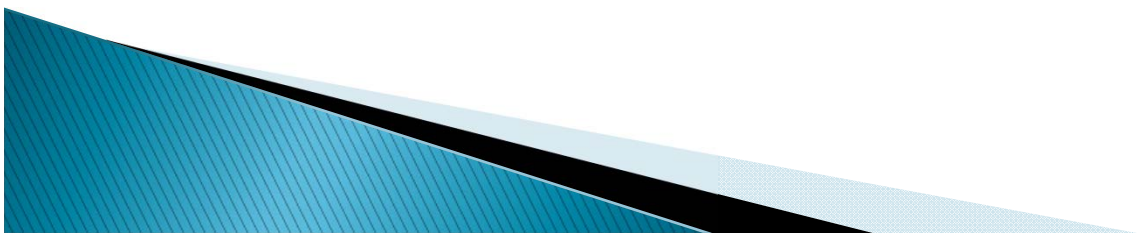

- We now turn to the quantum realm by invoking the third postulate of quantum mechanics, which states that every observable of a physical system is associated with a **Hermitian operator** with a complete set of eigenfunctions.
- The linear momentum and the particle position must then be replaced by the following operators: i ,ˆ .
- Therefore, the operator form of Eq. (6) becomes $E\ t$, $\hat{E}\ \hat{\imath}\ t\ i\ t$, where the operator product (ˆ / t) is given byˆ t (x , ,) ($\Sigma\ x\ t$, $\Sigma\ t$, $\Sigma\ t$) .
- We have proved that the operator i (/ t) represents the total energy of the quantum system. In doing so, **we never needed to think of time as an operator**.