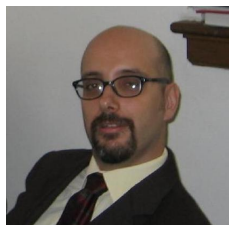


STEFANO CURTAROLO

CURRICULUM VITAE ET STUDIORUM

(December 11, 2014)

I. CONTACTS



Stefano Curtarolo, Ph.D.

Director, Center for Materials Genomics
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Department of Mechanical Engineering and Materials Science
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updated curriculum vitae: <http://materials.duke.edu/auro/cv.pdf>
Google Scholar : <http://scholar.google.com/citations?user=zuFUb-YAAAAJ>

II. SELECTED HYPERLINKS

[Education](#) - [Awards](#) - [Press Releases](#) - [Publications](#) - [Outreach](#)

III. ACADEMIC POSITIONS

- **Duke University**, Durham, NC, USA
 -) Director, Center for Materials Genomics, Pratt School of Engineering.
May 2012 - present.
 -) Professor of Materials Science, Electrical Engineering, Chemistry and Physics.
November 2013 - present (Full Prof. Electrical Engineering and Chemistry);
February 2012 - present (Full Prof. Materials Science and Physics);
October 2008 - February 2012 (Associate Prof. Materials Science and Physics);
September 2003 - October 2008 (Assistant Prof. Materials Science);
Appointments: Mechanical Eng. and Materials Science (primary) and Physics/Chemistry/Electrical Engineering (secondary).

IV. AWARDS AND HONORS

- Most downloaded article of Computational Materials Science in the last 90 days, in February 2014:
"Setyawan and Curtarolo, *High-throughput electronic band structure calculations: Challenges and tools*,
Comp. Mat. Sci. **49**(2), 299-312 (2010)"
- 2013 **Fellow of the American Physical Society** - Division of Computational Physics: *for automatic high-throughput computational materials science, and for the creation of on-line materials development techniques.*
- 2013 **DOD-MURI Award, 8.6M\$** as PI, *Topological decompositions and spectral sampling algorithms for element substitution in critical technologies*, Duke University, UMD, UNT, CMU, BYU.
- 2013 **Stansell Distinguished Research Award**, Duke University.

- 2012 **Invited Review in Nature Materials**, S. Curtarolo *et al.*, Nat. Mater. **12**, 191 (2013).
- 2011 **IUPAP Young Scientist Prize** in Computational Physics: *for pioneering high-throughput combinatorial computational materials science, for the creation of on-line materials development techniques, and for the development of thermodynamic models for nano-catalysts.* [[link](#)]
- 2011 **Fellow** of the Institute of Physics (IOP).
- 2009 Cover for Physical Review Letters **103**(5): *C₆₀ molecules (green) adsorbed in vacancy sites on a silver 111 surface (blue).* See also *Viewpoint in Physics and Editors' Suggestions.*
- 2009 Feinberg Foundation Visiting Faculty Program Fellowship, **Weizmann Institute.**
- 2007 **PECASE** Presidential Award: Department of Defense - Office of Naval Research (DoD-ONR, 1M\$ award) Awarded Dec. 2008.
- 2007 **NSF CAREER** Award: *Genetic Approaches to Quantum Mechanics Predictions of Materials Structures.*
- 2007 **ONR YIP** Award: *High-throughput ab initio combinatorial materials characterization of oxidation resistant titanium alloys and novel boride superconductors.*
- 2009. The paper H. I. Li *et al.*, Surface geometry of C₆₀ on Ag(111), Phys. Rev. Lett. **103**, 056101 (2009) was selected for "Editor Suggestions" in Volume **103** of PRL, and featured in the Viewpoint G. Held, *Nanospheres on a silver plate*, Physics **2**, 64 (2009).
- The paper R. V. Chepulskii and S. Curtarolo, First-principle solubilities of alkali and alkaline earth metals in Mg-B alloys, Phys. Rev. B **79**, 134203 (2009) was selected for "Editor Suggestions" in Volume **79** of PRB.
- The paper W. Setyawan *et al.*, Noble gases films on decagonal Al-Ni-Co quasicrystal surfaces, J. Phys.: Condens. Matter **19**, 016007 (2007) was selected for "IOP Select" based on 1) substantial advances or significant breakthroughs, 2) high degree of novelty, and 3) significant impact on future research.
- **Best paper published in 2005 in CALPHAD:** *Accuracy of ab initio methods in predicting the crystal structures of metals: A review of 80 binary alloys*, Volume 29, 2005, Pages 163-211, by Stefano Curtarolo, Dane Morgan and Gerbrand Ceder (2005).
- Most downloaded article of Calphad for the period October - December 2005. The article "Curtarolo *et al.*, *Accuracy of ab initio methods in predicting the crystal structures of metals: A review of 80 binary alloys*, Calphad **29**(3), 163-211 (2005)", was the most downloaded article of Calphad for the last quarter of 2005: http://top25.sciencedirect.com/index.php?cat_id=6&subject_area_id=15&journal_id=03645916
- Materials Research Society (**MRS**) **Silver Medal Graduate Student** Award (2002).
- American Physical Society Student Award funded by DOE and NSF (1999).
- Fondazione Gini Fellowships (1997, 1998, 1999).
- Penn State University Duncan Fellowship Award (1998 / 1999).
- Winner of the competition for a doctoral position in the Photonics and Optoelectronics Group, Department of Electronics Engineering (DEI), University of Padova (1995).

V. EDUCATION

- **Ph.D.: Massachusetts Institute of Technology**, Cambridge, MA USA.
Ph.D. Department of Materials Science and Engineering, August 2003.
Thesis: *Coarse-Graining and Data Mining Approaches to the Prediction of Structures and their Dynamics.*
Advisor: Gerbrand Ceder
- **MS: Pennsylvania State University**, State College, PA USA.
Master of Science in Physics. Department of Physics, August 1999.
Thesis: *Adsorption problems investigated with computer simulation.*
Advisor: Milton Cole

- **Laurea: University of Padova**, Padova, Italy.
Laurea in Physics (MS+BS) Magna cum Laude. Department of Physics, July 1998.
Thesis: *Roughness effect on prewetting of Ne on Mg*.
Advisor: Attilio Stella. 110/110 magna cum laude.
- **Laurea: University of Padova**, Padova, Italy.
Laurea in Electronics and Telecommunication Engineering (MS+BS).
Department of Electronics Engineering, July 1995.
Thesis: *Dielectric adiabatic tapers (Photonics)*.
Advisor: Carlo Giacomo Someda. 110/110.

VI. RESEARCH FIELDS

- Nanoscale Science of Energy
- Computational materials science
- Nanotube growth characterization (Honda R&I)
- Alloy theory (ONR-YIP Award 2007, NSF-CAREER Award 2007)
- Superlubricity on quasicrystals (ACS-PRF, NSF-DMR)
- Metal borides and related superconductors (ONR-YIP Award 2007)
- Genetic Approaches to QM Predictions of Materials Structures (NSF-Career Award 2007)

VII. ADVISING EXPERIENCE

- **Current Graduate Students:** Mr. David Hichs (2014-present) Mr. Corey Oses (2014-present)
- **Graduated Ph.D. and M.S. Students:** Dr. Junkai Xue (M.S. 2010-2011, Ph.D 2011-2013). Dr. Richard Taylor (M.S. 2010-2012, Ph.D. 2013). Dr. Wahyu Setyawan (Ph.D. 2004-2008). Dr. Neha Aswasthi (Ph.D. 2004-2007).
- **Postdocs and Research Professors:** Dr. Kesong Yang (2010-2013, Assistant Prof. of Nanoengineering, UCSD), Dr. Shidong Wang (2010-2013), Dr. Camilo E. Calderon (2012-present), Dr. Cormac Toher (2013-present), Dr. Allison Stelling (2013-present), Dr. Jose J. Plata (2013-present), Dr. Kevin Rasch (2013-2014), Dr. Demet Usanmax (2013-present), Dr. Pinku Nath (2014-present), Dr. Frisco Rose (2014-present), Dr. Junkai Xue (2013-2013), Dr. Cheng-Ing Chia (2012-2013), Dr. Wahyu Setyawan (2008-2011, Research Scientist, Pacific Northwest National Laboratory), Dr. Roman Chepulskyy (2007-2010, Samsung), Dr. San-Huang Ke (2008-2009), Dr. Aiqin Jiang (2006-2008), Dr. Aleksey Kolmogorov (2005-2008, Assistant Prof. of Physics at SUNY, Binghamton).
- **International/Exchange Students:** Ms. Anna Hirsch (Ph.D. student, Wiezmann Institute of Science, 2012-2013). Mr. Felipe Cervantes-Sodi (Ph.D. from Cambridge University, 2007-2008).
- **Duke Thesis Committee Students:** Manav Vohra (2013), Gianluca Di Muro (2011), Chandrasekhar Annavarapu (2010), Wishsanuruk Wechsattol (2005), Alexandre da Silva (2004).

VIII. RESEARCH EXPERIENCE

- **Duke University, Department of Mechanical Engineering and Materials Science**
Durham, NC. August 2003. *Research field: Theoretical materials science:* computational materials science, nanotube growth characterization (from metal alloy nanoparticles), alloy theory (data mining and high-throughput), gas adsorption in nanopatterned surfaces and nanoparticles (surface ordering of adsorbed films), superlubricity on quasicrystals (surface properties), metal borides and related superconductors (new phases and critical temperatures).
- **MIT, Department of Materials Science & Engineering**
Cambridge, MA. September 1999 - August 2003. Advisor: Prof. Gerbrand Ceder.
Research field: Materials modeling. Develop models for dynamics of inhomogeneous systems, based on renormalization of information.

- **Penn State University, Physics Department**

State College, PA. January 1998 - August 1999. Advisor: Prof. Milton Cole.

Research field: Statistical mechanics, Adsorption, Carbon NanoTubes. Developed computational tools for calculation of adsorption and wetting of gases on weak interfaces. Found first computations example of known pre-wetting transitions, predicted by theory. Found effect of surface roughness on adsorption properties of these systems. Developed model for adsorption of hydrogen gas inside Carbon Nanotubes.

- **University of Padova, Department of Electronics Engineering**

Padova, Italy. July 1994 - July 1995. Advisor: Carlo Giacomo Someda.

Research field: Optoelectronics. Developed computational tools to address losses in fiber-to-device optical adapters. Found evidence that adapters with minimum losses can be built by tailoring the refractive indices profile.

IX. TEACHING EXPERIENCE

- **Duke-University, Dept. Mech. Eng. & Material Science, Durham, NC.**

FA2011, *Intermediate Materials Science*, (grad level), lecturer.

FA2006, *Theory and calculations of Superconductivity*, (grad-research workshop), workshop organizer.

FA2010, FA2008, FA2006, FA2005, FA2004 *Structure and Properties of Solids*, (undergrad level), lecturer.

SP2012, SP2011, SP2008, SP2006, SP2005, SP2004, *Introduction to Solid State Engineering*, (grad level), lecturer.

SP2007, *Solid State Engineering II*, (grad level), lecturer.

- **MIT Department of Material Science & Engineering, Cambridge, MA. (Fall 2001).;** *Electronic,*

Magnetic and Optical Properties of Materials. Lecturer and teaching assistant. Lectured part of the course, taught recitations, prepared exams, and problem sets.

- **Penn State University, Physics Department, State College, PA. (Spring 1999).** Teaching Assistant:

taught recitations, prepared exams, and problem sets.

- **University of Padova, Measurements Laboratory. Italy. (Spring 1992).**

Teaching Assistant: taught Electric Measurements Laboratory techniques and developed tools for automatic data acquisition.

X. OUTREACH AND PROFESSIONAL ACTIVITIES

- Advisory Programming Committee, Foundations of Molecular Modeling and Simulation, FOMMS (2015).
- Organizer EMRS2014 Symposium BB, Materials by design for energy applications through theory and experiment (2014).
- Duke University, Academic Council elected member (2014-2017).
- International Advisory Board Member: Conference on Computational Physics (CCP2012).
- Member: IOP, APS (DCMP, DCOMP, DMP, FIAP, FPS, SESAPS), MRS, TMS, ACS, ASME.
- Organizer and Chair of the Symposium BB: *Materials by design for energy applications through theory and experiment*, EMRS Spring Meeting 2014.
- Organizer and Chair of the Symposium NN: *Strategies and Techniques to Accelerate Inorganic Materials Innovation*, MRS Fall Meeting 2013.
- Co-presenter of educational outreach: *Science Go Round*, J.Y. Joyner Elementary School, Raleigh, NC, February 18, 2011.
- Chair of the *Focus Session: Frontiers in Computational Thermodynamics of Materials*, American Physical Society March Meeting, 2011.
- Organizer and Chair of the Symposium II: *Theory and Computer Simulation of Materials* at the XIX International Materials Research Congress, Mexico, 2010.
- Organizer and Chair of the *Focus Session: Frontiers in Computational Thermodynamics of Materials*, American Physical Society March Meeting, 2010.
- Organizer and Chair of the Symposium II: *Theory and Computer Simulation of Materials* at the XVIII International Materials Research Congress, Mexico, 2009.
- Chair of the Session: *Discovery and Optimization of Materials through Computational Design* at Materials Science & Technology Conference, Pittsburgh, 2008.
- Co-organizer and Co-chair of the Symposium: *Theory and Computer Simulation of Materials* at the XVII International Materials Research Congress, Mexico, 2008.
- Chair of the Session: *Phase Stability and Phase Transitions* at the American Physical Society March Meeting, 2008.
- Chair of the Session: *Composite and Porous Media* at the American Physical Society March Meeting, 2008.
- Co-organizer and Co-chair of the Symposium: *Theory and Computer Simulation of Materials* at the XVI International Materials Research Congress, Mexico, 2007.
- Chair of the Symposia: *Carbon Nanotubes: Superconductivity* and *Metals: Alloys and Compounds* at the American Physical Society March Meeting, 2007.
- Co-organizer and Co-chair of the Symposium: *Theory and Computer Simulation of Materials* at the XV International Materials Research Congress, Mexico, 2006.
- Organizer and chair of the Symposium: *Frontiers of Computational Materials* at the American Physical Society March Meeting, 2006.
- Chair of the Session: *Quasicrystals, Adsorption on Quasicrystals, Porous and Random Materials* at the American Physical Society March Meeting, 2006.
- Journal referee for *ACS Nano*, *Advanced Materials*, *Advanced Functional Materials*, *Calphad*, *Carbon*, *Computational Materials Science*, *Energy & Environmental Science*, *Intermetallics*, *Journal of Alloys and Compounds*, *Journal of American Chemical Society*, *Journal of Materials Science*, *Journal of Physical Chemistry*, *Journal of Physics: Condensed Matter*, *Langmuir*, *Nature*, *Nature Materials*, *Nature Communications*, *MRS Communications*, *Physical Review Letters*, *Physical Review B*, *Physical Review E*, *Physical Review X*, *Science*, *Surface Science*.

- Proposal Referee for NSF, DOE, ONR, AFOSR, NASA, and ACS (PRF).
- Panelist for NSF: Division of Materials Research.
- Panelist for NSF: Office of Cyberinfrastructure.

XI. PRESS AND NEWS RELEASES


- Duke University, 2014/01/03,
Supercomputers Join Search for “Cheapium:” Duke Engineers Use Brute Force Computing to Find New Materials.
<http://www.pratt.duke.edu/node/4561>
- Duke University, 2012/05/13,
“KeyGenetic Search of Novel Electrical Crystals.
<http://www.pratt.duke.edu/node/3256>
- Duke University, 2011/11/29,
New Elemental Cookbook Guides Efficient Thermoelectric Combinations.
<http://www.pratt.duke.edu/node/3196>
- Duke University, 2010/11/17,
New Technology Gives On-Site Assessments in Archaeology.
http://www.pratt.duke.edu/duke_curarolo_calcite
- Duke University, 2010/10/21,
Smaller is Better in the Viscous Zone.
http://www.pratt.duke.edu/duke_curtarolo_nano
- Duke University, 2006/05/08,
New “Metal Sandwich” May Break a Superconductor Record, Theory Suggests.
<http://dukenews.duke.edu/2006/05/superconductor.html>
- Duke University, 2005/09/15,
DUKE-PSU Researchers Aim for UltraLow-Friction Machine Parts with Computer Model of Quasicrystal Metal.
<http://www.dukenews.duke.edu/2005/09/quasicrystals.html>
- Massachusetts Institute of Technology, 2003/11/17,
MIT team mines for new materials with a computer.
<http://web.mit.edu/newsoffice/2003/datamining.html>

XII. PATENTS

- G. Ceder, C. Fischer, K. Tibbetts, D. Morgan, S. Curtarolo, *Systems and Methods for predicting materials properties*, US Patent

XIII. PUBLICATIONS

[Articles can be accessed through the embedded link. Only published, submitted and “in press” articles are listed. The list might be slightly out of order.]


100. M. de Jong, W. Chen, T. Angsten, A. Jain, R. Notestine, A. Gamst, M. Sluiter, C. Ande, S. van der Zwaag, S. Curtarolo, C. Toher, J. J. Plata, G. Ceder, K. Persson, and M. D. Asta, *Charting the Complete Elastic properties of Inorganic Crystalline Compounds*, submitted (2014).
99. C. M. Rost, E. Sachet, T. Borman, A. Moballeghe, E. C. Dickey, D. Hou, J. L. Jones, S. Curtarolo, and J.-P. Maria, *Infrared excitons in refractory systems*, submitted (2014).
98. J. Yong, Y. Jiang, D. Usanmaz, S. Curtarolo, X. Zhang, L. Li, X. Pan, J. Shin, I. Tachuchi, and R. L. Greene, *Robust topological surface state in Kondo insulator SmB_6 thin films*, Appl. Phys. Lett. **105**, 222403 (2014).
DOI: [10.1063/1.4902865](https://doi.org/10.1063/1.4902865)
97. E. Sachet, C. T. Shelton, J. S. Harris, B. E. Gaddy, D. L. Irving, S. Curtarolo, B. F. Donovan, P. E. Hopkins, P. A. Sharma, A. Lima Sharma, J. Ihlefeld, S. Franzen, and J.-P. Maria, *Dysprosium doped cadmium oxide: A gateway material for mid-infrared plasmonics*, in press, Nature Materials **VV**, PP (2014).
96. C. Toher, J. J. Plata, O. Levy, M. de Jong, M. D. Asta, M. Buongiorno Nardelli, and S. Curtarolo, *High-throughput computational screening of thermal conductivity, Debye temperature, and Grüneisen parameter using a quasiharmonic Debye model*, Phys. Rev. B **90**, 174107 (2014).
DOI: [10.1103/PhysRevB.90.174107](https://doi.org/10.1103/PhysRevB.90.174107)
95. J. Carrete, N. Mingo, and S. Curtarolo, *Low thermal conductivity and triaxial phononic anisotropy of $SnSe$* , Appl. Phys. Lett. **105**, 101907 (2014).
DOI: [10.1063/1.4895770](https://doi.org/10.1063/1.4895770)
94. O. Isayev, D. Fourches, E. N. Muratov, C. Oses, K. Rasch, A. Tropsha, and S. Curtarolo, *Materials Cartography: Representing and Mining Material Space Using Structural and Electronic Fingerprints*, in press, Chem. Mater. **VV**, PP (2014).
93. L. A. Agapito, S. Curtarolo, and M. Buongiorno Nardelli, *Reformulation of DFT+U as a pseudo-hybrid Hubbard density functional for accelerated materials discovery*, submitted (2014). [[pdf](#)]
92. R. H. Taylor, F. Rose, C. Toher, O. Levy, K. Yang, M. Buongiorno Nardelli, and S. Curtarolo, *A RESTful API for exchanging materials data in the AFLOWLIB.org consortium*, Comp. Mat. Sci. **93**, 178-192 (2014).
DOI: [10.1016/j.commatsci.2014.05.014](https://doi.org/10.1016/j.commatsci.2014.05.014)
91. A. Hirsch, I. Azuri, L. Addadi, S. Weiner, K. Yang, S. Curtarolo, and L. Kronik, *Infrared Absorption Spectrum of Brushite from First Principles*, Chem. Mater. **26**(9), 2934-2942 (2014).
DOI: [10.1021/cm500650t](https://doi.org/10.1021/cm500650t)
90. M. Mehl, D. Finkenstadt, C. Dane, G. L. W. Hart, and S. Curtarolo, *First-principles study of the phase diagram of Tungsten Nitride*, submitted (2014). [[pdf](#)]
89. E. Martínez-Guerra, F. Ortíz-Chi, S. Curtarolo, and R. de Coss, *Pressure effects on the electronic structure and superconducting critical temperature of Li_2B_2* , J. Phys.: Condens. Matter **26**, 115701 (2014).
DOI: [10.1088/0953-8984/26/11/115701](https://doi.org/10.1088/0953-8984/26/11/115701)
88. J. Petucci, M. Karimi, Y.-T. Huang, S. Curtarolo, and R. D. Diehl, *Ordering and growth of rare gas films (Xe , Kr , Ar , and Ne) on the ten-fold quasicrystalline approximant $Al_{13}Co_4(100)$ surface*, J. Phys.: Condens. Matter **26**, 095003 (2014).
DOI: [10.1088/0953-8984/26/9/095003](https://doi.org/10.1088/0953-8984/26/9/095003)
85. J. Carrete, N. Mingo, S. Wang, and S. Curtarolo, *Nanograined half-Heusler semiconductors as advanced thermoelectrics: an ab-initio high-throughput statistical study*, Adv. Funct. Mater. doi=10.1002/adfm.201401201 (2014).
DOI: [10.1002/adfm.201401201](https://doi.org/10.1002/adfm.201401201)
84. J. Carrete, W. Li, N. Mingo, S. Wang, and S. Curtarolo, *Finding unprecedentedly low-thermal-conductivity half-Heusler semiconductors via high-throughput materials modeling*, Phys. Rev. X **4**, 011019 (2014).
DOI: [10.1103/PhysRevX.4.011019](https://doi.org/10.1103/PhysRevX.4.011019)
87. G. L. W. Hart, S. Curtarolo, T.B. Massalski, and O. Levy, *Comprehensive Search for New Phases and Compounds in Binary Alloy Systems Based on Platinum-Group Metals, Using a Computational First-Principles Approach*, Phys. Rev. X **3**, 041035 (2013).
DOI: [10.1103/PhysRevX.3.041035](https://doi.org/10.1103/PhysRevX.3.041035) 
Viewpoint, M. Fornari, *Computational Materials Discovery Goes Platinum*, Physics **6**, 140 (2013). [[DOI: 10.1103/Physics.6.140](https://doi.org/10.1103/Physics.6.140)]
86. L. A. Agapito, A. Ferretti, A. Calzolari, S. Curtarolo, and M. Buongiorno Nardelli, *Effective and accurate representation of extended Bloch states on finite Hilbert spaces*, Phys. Rev. B **88**, 165127 (2013).
DOI: [10.1103/PhysRevB.88.165127](https://doi.org/10.1103/PhysRevB.88.165127)

83. M. Gascón, S. Lam, S. Wang, S. Curtarolo, and R. S. Feigelson, *Characterization of light output and scintillation emission in CsI(Tl), NaI(Tl), and LaBr₃(Ce) under isostatic pressure*, Radiation Measurements, **56**, 70-75 (2013).
DOI: [10.1016/j.radmeas.2013.04.017](https://doi.org/10.1016/j.radmeas.2013.04.017)
82. R. Rao, N. Pierce, D. Liptak, D. Hooper, G. Sargent, S. L. Semiatin, S. Curtarolo, A. R. Harutyunyan, and B. Maruyama, *Revealing the Impact of Catalyst Phase Transition on Carbon Nanotube Growth by In Situ Raman Spectroscopy*, ACS Nano **7**(2), 1100-1107 (2013).
DOI: [10.1021/nn304064u](https://doi.org/10.1021/nn304064u)
81. S. Curtarolo, G. L. W. Hart, M. Buongiorno Nardelli, N. Mingo, S. Sanvito, and O. Levy, *The high-throughput highway to computational materials design*, Nature Materials **12**(3), 191-201 (2013).
DOI: [10.1038/nmat3568](https://doi.org/10.1038/nmat3568)
Note. This paper was featured in *Nature Materials*, Volume **12**(3).
Editorial. *Fuelling discovery by sharing*, Nature Materials **12**(3), 173 (2013). [DOI: [10.1038/nmat3594](https://doi.org/10.1038/nmat3594)]
79. S. Lam, M. Gascón, S. Podowitz, S. Curtarolo, and R. S. Feigelson, *Nonproportionality and Scintillation Studies of LSO:Ce From 4.3 to 300 K*, IEEE Trans. Nucl. Sci. **60**(2), 993-999.
DOI: [10.1109/TNS.2012.2234136](https://doi.org/10.1109/TNS.2012.2234136)
78. R. M. Gaumé, S. Lam, M. Gascón, W. Setyawan, S. Curtarolo, and R. S. Feigelson, *An apparatus for studying scintillator properties at high isostatic pressures*, Rev. Sci. Instrum. **84**, 015109 (2013).
DOI: [10.1063/1.4773563](https://doi.org/10.1063/1.4773563)
80. G. S. Rohrer, M. Affatigato, M. Backhaus, R. K. Bordia, H. M. Chan, S. Curtarolo, A. Demkov, J. N. Eckstein, K. T. Faber, J. E. Garay, Y. Gogotsi, L. Huang, L. E. Jones, S. V. Kalilin, R. J. Lad, C. G. Levi, J. Levy, J.-P. Maria, L. Mattos Jr., A. Navrotsky, N. Orlovskaya, C. Pantano, J. F. Stebbins, T. S. Sudarshan, T. Tani, and K. S. Weil, *Challenges in Ceramic Science: A Report from the Workshop on Emerging Research Areas in Ceramic Science*, J. Am. Ceram. Soc., **95**(12) 3699-3712 (2012).
DOI: [10.1111/jace.12033](https://doi.org/10.1111/jace.12033)
77. K. Yang, W. Setyawan, S. Wang, M. Buongiorno Nardelli, and S. Curtarolo, *A search model for topological insulators with high-throughput robustness descriptors*, Nature Materials **11**(7), 614-619 (2012).
DOI: [10.1038/nmat3332](https://doi.org/10.1038/nmat3332)
76. W.-C. Wen, R. V. Chepulsii, L.-W. Wang, S. Curtarolo, and C.-H. Lai, *Accelerating disorder-order transitions of FePt by preforming a metastable AgPt phase*, Acta Mat. **60**(20), 7258-7264 (2012).
DOI: [10.1016/j.actamat.2012.09.045](https://doi.org/10.1016/j.actamat.2012.09.045)
75. S. Curtarolo, W. Setyawan, S. Wang, J. Xue, K. Yang, R. H. Taylor, L. J. Nelson, G. L. W. Hart, S. Sanvito, M. Buongiorno Nardelli, N. Mingo, and O. Levy, *AFLOWLIB.ORG: a distributed materials properties repository from high-throughput ab initio calculations*, Comp. Mat. Sci. **58**, 227-235 (2012).
DOI: [10.1016/j.commatsci.2012.02.002](https://doi.org/10.1016/j.commatsci.2012.02.002)
74. J. Bloch, O. Levy, B. Pejova, J. Jacob, S. Curtarolo, and B. Hjörvarsson, *Prediction and hydrogen-acceleration of ordering in iron-vanadium alloys*, Phys. Rev. Lett. **108**, 215503 (2012).
DOI: [10.1103/PhysRevLett.108.215503](https://doi.org/10.1103/PhysRevLett.108.215503)
73. S. Lam, M. Gascón, R. Hawrami, W. Setyawan, S. Curtarolo, R. S. Feigelson, and R. M. Gaumé, *Nonproportionality and Scintillation Studies of Eu:SrI₂ From 295 to 5K*, IEEE Trans. Nucl. Sci. **58**(5), 2052-2056 (2012).
DOI: [10.1109/TNS.2012.2186317](https://doi.org/10.1109/TNS.2012.2186317)
71. L. J. Nelson, G. L. W. Hart, and S. Curtarolo, *Ground state characterizations of systems predicted to exhibit L1₁ or L1₃ crystal structures*, Phys. Rev. B **85**, 054203 (2012).
DOI: [10.1103/PhysRevB.85.054203](https://doi.org/10.1103/PhysRevB.85.054203)
70. O. Levy, J. Xue, S. Wang, G. L. W. Hart, and S. Curtarolo, *Stable ordered structures of binary technetium alloys from first principles*, Phys. Rev. B **85**, 012201 (BR) (2012).
DOI: [10.1103/PhysRevB.85.012201](https://doi.org/10.1103/PhysRevB.85.012201)
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