Materials Project User's articles

1.Battery

(1) Computational screening of perovskite metal oxides for optimal solar light capture†

Description: Ivano E. Castelli et al. studied new photoelectrochemical cells which can absorb light more effectively. Those highly effective light-absorption materials should have bandgaps to absorb a large part of the solar spectrum. They screened 5400 different materials, relevant oxide and oxynitride materials, to find promising candidates, 15 materials having been found in the end.

Materials Genome Project: They used Materials Genome and ICSD databases to expand their reference systems, querying bulk metals and most stable single- and bi-metal oxides in their equilibrium structures.

Ivano E. Castelli, Thomas Olsen, Soumendu Datta, David D. Landis, Sren Dahl, Kristian S. Thygesen, and Karsten W. Jacobsen (2012). Computational screening of perovskite metal oxides for optimal solar light capture. Energy Environ. Sci. 5(2). doi:10.1039/c1ee02717d

Cited by 243

(2) Alloy Negative Electrodes for High Energy Density Metal-Ion Cells

Description: Tuan T. Tran et al. studied the volume expansion behavior and volumetric energy densities of metal alloy cathode materials (A_xM). They compared different metal A: Li, Na, K, Ca and Al and found that both Mg_xM, Al_xM showed high energy densities over all known Li-ion cathode materials based on prediction.

Materials Genome Project: voltage prediction at 0K by the Materials Genome Project.

Tuan T. Tran and M. N. Obrovac (2011). Alloy Negative Electrodes for High Energy Density Metal-Ion Cells. Journal of The Electrochemical Society 158(12). doi: 10.1149/2.083112jes

Cited by 54

(3) Holistic computational structure screening of more than 12000 candidates for solid lithium-ion conductor materials†

Description: Austin D. Sendek et al. presented a new type of large-scale computational screening approach for identifying promising candidate materials for solid state electrolytes for lithium ion batteries. They screened 12831 lithium containing crystalline solids for those desirable characteristics, such as high structural and chemical stability, low electronic conductivity etc.

Materials Project: All those screening structures and electronic information contained in the Materials Project database.

Austin D. Sendek, Qian Yang, Ekin D. Cubuk, Karel-Alexander N. Duerloo, Yi Cui, and Evan J. Reed (2017). Holistic computational structure screening of more than 12\hspace0.167em000 candidates for solid lithium-ion conductor materials. Energy Environmental Science 10(1). doi:10.1039/c6ee02697d

Cited by 49

(4) Titanate Anodes for Sodium Ion Batteries

Description: Marca M.Doeff studied rechargeable sodium ion batteries. Selection of the anode material is the critical challenge. In this paper, a brief overview of most promising materials for sodium-ion battery applications is given, and a comparison is made between the sodium and the lithium insertion behavior.

Materials Projects: They utilized Materials Project to obtain Na-Ti-O ternary phase diagram.

Marca M. Doeff, Jordi Cabana, and Mona Shirpour (2013). Titanate Anodes for Sodium Ion Batteries. Journal of Inorganic and Organometallic Polymers and Materials 24(1). doi:10.1007/s10904-013-9977-8

Cited by 47

(5) Combinatorial Studies of Si1−xOx as a Potential Negative Electrode Material for Li-ion Battery Applications

Description: M.A.Al-Maghrabi et al. studied the approach to obtain the desired specific capacity of negative electrode in Li-ion and showed oxygen content in $Si_{1-x}O_x$ should be optimized to get such desired specific capacity.

Materials Project: They utilized materials project to obtain Li-Si-O ternary phase diagram.

M. A. Al-Maghrabi, J. Suzuki, R. J. Sanderson, V. L. Chevrier, R. A. Dunlap, and J. R. Dahn (2013). Combinatorial Studies of Si1-xOx as a Potential Negative Electrode Material for Li-Ion Battery Applications. Journal of the Electrochemical Society 160(9). doi: 10.1149/2.115309jes

Cited by 41

(6) Phase stability of Li–Mn–O oxides as cathode materials for Li-ion batteries: insights from ab initio calculations†

Description: R.C. Longo worked on examing phase stability, electrochemical stability and phase transformation mechanism of the layered and over-lithiated Mn oxides based on density functional theory. They also used a thermodynamic model analysis to found the requirement temperature for oxygen evolution and Li vacancy formation is over than any synthesis temperature. Meantime, they utilized solid-state transition calculations to identify the key steps in the phase transition mechanism.

Materials Project: They took the initial structures for each compound from the materials project database.

R. C. Longo, F. T. Kong, Santosh KC, M. S. Park, J. Yoon, D.-H. Yeon, J.-H. Park, S.-G. Doo, and K. Cho (2014). Phase stability of Li-Mn-O oxides as cathode materials for Li-ion batteries: insights from ab initio calculations. Phys. Chem. Chem. Phys. 16(23). doi:10.1039/c4cp00937a

Cited by 37

(7) Application of machine learning methods for the prediction of crystal system of cathode materials in lithium-ion batteries

Description: M. Attarian Shandiz et al. showed an approach based on machine learning to predict the crystal systems of silicate-based cathodes with Li-Si-(Mn,Fe,Co)-O compositions

Materials Project: the calculations are based on the results of density functional theory calculations from Material Project.

M. Attarian Shandiz and R. Gauvin (2016). Application of machine learning methods for the prediction of crystal system of cathode materials in lithium-ion batteries. Computational Materials Science. doi:10.1016/j.commatsci.2016.02.021

Cited by 11

2. Insulator/Semiconductor/conductor materials

(1) Identifying defect-tolerant semiconductors with high minority-carrier lifetimes: beyond hybrid lead halide perovskites

Description: Riley E.Brandt et al. studied the emergence of methyl-ammonium lead halide($MAPbX_3$) perovskites which motivates the identification of unique properties giving rise to exceptional bulk transport properties, and identifying future materials with similar properties.

Materials Project: To identify promising materials in this class, they developed a script to search through all materials in the Materials project.

Riley E. Brandt, Vladan Stevanovi, David S. Ginley, and Tonio Buonassisi (2015). Identifying defect-tolerant semiconductors with high minority-carrier lifetimes: beyond hybrid lead halide perovskites. Communications 5(02). doi:10.1557/mrc.2015.26

Citied by 277

(2) How Does Chemistry Influence Electron Effective Mass in Oxides? A High-Throughput Computational Analysis

Description: Geoffeoy Hautier et al. studied high electronic conductivity or mobility of oxides based on screening over 4000 binary and ternary oxides to identify compounds which have lowest electron effective mass. They found 74 promising oxides and suggest a few novel potential n-type transparent conducting oxides with large band gap and low effective mass.

Materials Project: they evaluated the line electron effective mass for binary and ternary oxides present in the Materials project database.

Geoffroy Hautier, Anna Miglio, David Waroquiers, Gian-Marco Rignanese, and Xavier Gonze (2014). How Does Chemistry Influence Electron Effective Mass in Oxides? A High-Throughput Computational Analysis. Chemistry of Materials 26(19). doi:10.1021/cm404079a

Cited by 64

(3) Comprehensive examination of dopants and defects in BaTiO3 from first principles

Description: V.Sharma et al. assessed the factors manipulating the behavior of dopant-related defects in $BaTiQ_3$, which leveraged high-throughput first-principles computations. They traversed the 44 elements from periodic table showing that the most prominent factor that controls dopant stability in $BaTiO_3$is the dopant ionic size.

Materials Project: They leveraged Materials Project to query the formation energies of 45 stable simple oxides.

V. Sharma, G. Pilania, G. A. Rossetti, K. Slenes, and R. Ramprasad (2013). Comprehensive examination of dopants and defects in BaTiO3from first principles. Physical Review B 87(13). doi:10.1103/physrevb.87.134109

Citied by 30

(4) Electronic structure and defect properties of B6O from hybrid functional and many-body perturbation theory calculations: A possible ambipolar transparent conductor

Description: J.B. Varley et al. studied the electronic structure and defect properties of B_6O using a combination of hybrid functional and many-body perturbation theory calculation.

Materials Project: They found the chemical potential limits for any extrinsic defect by competitive phases in the X-B-O-H phase diagram using the Materials Project database.

J. B. Varley, V. Lordi, A. Miglio, and G. Hautier (2014). Electronic structure and defect properties ofB6Ofrom hybrid functional and many-body perturbation theory calculations: A possible ambipolar transparent conductor. Physical Review B 90(4). doi:10.1103/physrevb.90.045205

Citied by 15

(5) High-throughput search of ternary chalcogenides for p-type transparent electrodes

Description: Jinming Shi et al. studied delafossite crystals screening 15624 compounds aiming to find stable trigonal delafossite prototype structures. They also claimed that there were 79 systems not present in the materials project database.

Materials Project: They screened compositions from Materials Project database.

Jingming Shi, Tiago F. T. Cerqueira, Wenwen Cui, Fernando Nogueira, Silvana Botti, and Miguel A. L. Marques (2017). High-throughput search of ternary chalcogenides for p-type transparent electrodes. Scientific Reports. doi:10.1038/srep43179

Citied by 11

(6) Pressure-induced structural changes and insulator-metal transition in layered bismuth triiodide, BiI3: a combined experimental and theoretical study

Description: T.R.Devidas et al. studied the influence on the structure, phonons and electronic properties of rhombohedral BiI_3. They discovered that a drop of resistivity of BiI_3 in the 1-3GPa may because the appearance of an intermediate crystal phase with a lower band-gap and hexagonal crystal structure.

Materials Project: They looked for lattice parameters for the rhombohedral structure on Material Projects database.

T R Devidas, N V Chandra Shekar, C S Sundar, P Chithaiah, Y A Sorb, V S Bhadram, N Chandrabhas, K Pal, U V Waghmare, and C N R Rao (2014). Pressure-induced structural changes and insulator-metal transition in layered bismuth triiodide, BiI3: a combined experimental and theoretical study. Journal of Physics: Condensed Matter 26(27). doi:10.1088/0953-8984/26/27/275502

Citied by 9

(7) Assessing the performance of the Tran–Blaha modified Becke–Johnson exchange potential for optical constants of semiconductors in the ultraviolet–visible light region

Description: Kousuke Nakano et al. reported the performance of DFT with Tran-Blaha modified Becke-Johnson exchange potential and the random phase approximation dielectric function for optical constants of semiconductors in the ultraviolet-visible light region.

Materials Project: They used compounds database from Materials Project and compare their calculation of bandgaps E_g with data from Materials Project where leveraged GGA-PBE exchange-correlation function.

Kousuke Nakano and Tomohiro Sakai (2018). Assessing the performance of the Tran-Blaha modified Becke-Johnson exchange potential for optical constants of semiconductors in the ultraviolet-visible light region. Journal of Applied Physics 123(1). doi:10.1063/1.5006170

3. Layered Materials

(1) Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials Michael

Michael Ashton et al. found 826 stable layered materials candidates for the formation of 2D monolayers via exfoliation. Density functional theory was used to calculate the exfoliation energy of each material and 680 monolayers which has lower exfoliation energies than those of already identified 2D materials.

Materials Project: They used crystal structure database embedded in Materials Project for their works.

Michael Ashton, Joshua Paul, Susan B. Sinnott, and Richard G. Hennig (2017). Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. Physical Review Letters 118(10). doi:10.1103/physrevlett.118.106101

Citied by 68

(2) Defect chemistry in layered transition-metal oxides from screened hybrid density functional calculations

Description: Khang Hoang et al. reported thermodynamics and transport of intrinsic point defects in layered oxide cathode materials LiMO2(M = Co, Ni), using density-functional theory and the HSE screened hybrid functional.

Materials Project: they calculated all possible Li-M-O phases available in Materials Project database.

Khang Hoang and Michelle D. Johannes (2014). Defect chemistry in layered transition-metal oxides from screened hybrid density functional calculations. J. Mater. Chem. A 2(15). doi:10.1039/c4ta00673a

Citied by 61

(3) Data Mining for New Two- and One-Dimensional Weakly Bonded Solids and Lattice-Commensurate Heterostructures

Description: Gowoon Cheon et al. focused on identification of layered materials using data mining algorithm that determines the dimensionality of weakly bonded subcomponents based on the atomic positions of three-dimensional crystal structures.

Materials Project: They used 50,000 inorganic crystals from Materials Project.

Gowoon Cheon, Karel-Alexander N. Duerloo, Austin D. Sendek, Chase Porter, Yuan Chen, and Evan J. Reed (2017). Data Mining for New Two- and One-Dimensional Weakly Bonded Solids and Lattice-Commensurate Heterostructures. Nano Letters 17(3). doi:10.1021/acs.nanolett.6b05229

Citied by 39

(4) High-throughput Identification and Characterization of Two- dimensional Materials using Density functional theory

Description: Kamal Choudhary introduced a criterion to identify two-dimensional materials based on the comparison between experimental lattice constants and lattices constants mainly obtained from Materials Project density functional theory calculation.

Materials Project: They applied 1356 possible 2D materials out of all the systems in the Materials Project database.

Kamal Choudhary, Irina Kalish, Ryan Beams, and Francesca Tavazza (2017). High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory. Scientific Reports 7(1). doi:10.1038/s41598-017-05402-0

Citied by 26

4. physical and chemical processing

(1) Density functional calculations of the enthalpies of formation of rare-earth orthophosphates†

Description: James R. Rustad's group put effort in electronic structure calculations to estimate the enthalpies of formation of rare earth orthophosphates from oxides. There is systematically less exothermic in the calculation. According to comparison of the electronic structure calculation utilization to calculate the enthalpies of formation of alkaline earth oxyacid carbonates, silicates, and sulfates, they found an approach to get more accurate result: studying the simpler oxyacids and then predict the enthalpies of formation of more complicate components.

Materials Project: They used Materials Genome Reaction Calculator database to found experimental data of ΔH^{f}_{ox}

J. R. Rustad (2012). Density functional calculations of the enthalpies of formation of rare-earth orthophosphates. American Mineralogist 97(5-6). doi:10.2138/am.2012.3948

Citied by 39

(2) Formation of amorphous phase with crystalline globules in Fe–Cu–Nb–B immiscible alloys

Description: Takeshi Nagase et al. discovered the microstructure of arc-melted ingots and rapidly solidified melt-spun ribbons of quaternary Fe-Cu-Nb-B immiscible alloys. They focused on amorphous-phase formation and solidification structure.

Materials Project: They showed quaternary phase diagram at 0 k for the Fe-Nb-B-Cu alloy constructed using first principles calculations from the Materials Project.

Takeshi Nagase, Masanori Suzuki, and Toshihiro Tanaka (2015) . Formation of amorphous phase with crystalline globules in Fe–Cu–Nb–B immiscible alloys Journal of Alloys and Compounds. doi:10.1016/j.jallcom.2014.08.229

Citied by 17

(3) Large scale in silico screening of materials for carbon capture through chemical looping†

Description: Cindy Y. Lau studied the materials can be used in Chemical looping combustion applying large scale in silico screening methods and aimed to discover candidate materials.

Materials Project: In their works, they leveraged Materials Project database and sought for novel carbon capture and storage materials, mainly the geometry optimized structures and ground state energies of those relevant materials using VASP. They implemented Hubbard U values optimized for oxidation energies of transition metal oxides which improved DFT-GGA calculations in the Materials Project.

Cindy Y. Lau, Matthew T. Dunstan, Wenting Hu, Clare P. Grey, and Stuart A. Scott (2017). Large scale in silico screening of materials for carbon capture through chemical looping. Energy Environmental Science 10(3). doi:10.1039/c6ee02763f

Citied by 11

(4) DFT-supported phase-field study on the effect of mechanically driven fluxes in Ni4Ti3 precipitation

Description: Reza Darvishi Kamachali et al. studied the formation of Ni4Ti3 precipitate using phase-field modelling and density functional theory calculation.

Materials Project: They utilized Materials Project as a reference to compare with their DFT results scanning all known structures in Ni-Ti binary phase diagram.

Reza Darvishi Kamachali, Efim Borukhovich, Nicholas Hatcher, and Ingo Steinbach (2014). DFT-supported phase-field study on the effect of mechanically driven fluxes in Ni4Ti3precipitation. Modelling and Simulation in Materials Science and Engineering 22(3). doi:10.1088/0965-0393/22/3/034003

Citied by 10

(5) Amorphous phase formation in Fe–Ag-based immiscible alloys

Description: Takeshi Nagase et al. studied the formation of an amorphous phase in (Fe-M-B)-Ag, where M = Si, Zr, Nb.

Materials Projects: They queried quaternary phase diagrams from the Materials Project based on first-principles calculations.

Takeshi Nagase, Masanori Suzuki, and Toshihiro Tanaka (2015). Formation of amorphous phase with crystalline globules in Fe-Cu-Nb-B immiscible alloys. Journal of Alloys and Compounds. doi:10.1016/j.jallcom.2014.08.229

Citied by 9

(6) Phase separation in Fe2CrSi thin films

Description: Markus Meinert et al. studied the decomposition of Fe_2CrSi thin films after heat treatment. The thin films decomposed into Fe_3Si with $D0_3$ structure and Cr_3Si with A15 structure, explaining the results using *ab initio* calculations.

Materials Project: They obtained the computational results of formation energies and binary decompositions from Materials Project database.

Markus Meinert, Torsten Habner, Jan Schmalhorst, Ganter Reiss, and Elke Arenholz (2013). Phase separation in Fe2CrSi thin films. Journal of Applied Physics 114(11). doi:10.1063/1.4821972

Citied by 5

(7) Investigation of Thorium Salts As Candidate Materials for Direct Observation of the 229mTh Nuclear Transition

Description: Jason K.Ellis et al. studied the electronic structure of wide-gap thorium salts from measuring the nuclear transition of $^{229m}Th \rightarrow {}^{229g}Th$.

Materials Project: They compared their calculate data with the GGA calculations using PBE functional preformed by the Materials Project.

Jason K. Ellis, Xiao-Dong Wen, and Richard L. Martin (2014). Investigation of Thorium Salts As Candidate Materials for Direct Observation of the 229mTh Nuclear Transition. Inorganic Chemistry 53(13). doi:10.1021/ic500570u

Citied by 4

5. Materials Properties

(1) First-principles study of luminescence in Eu^{2+}-doped inorganic scintillators

Description: A.Chaudhry et al. studied Eu^{2+} luminescence materials using theoretical calculations based on density functional theory. They also applied the previously criteria Ce-doped systems to new Eu-doped materials.

Materials Project: The Materials Project was used us a resource in this paper.

A. Chaudhry, R. Boutchko, S. Chourou, G. Zhang, N. Grnbech-Jensen, and A. Canning (2014). First-principles study of luminescence in Eu^{2+}-doped inorganic scintillators. Physical Review B 89(15). doi:10.1103/physrevb.89.155105

Citied by 56

(2) Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure

Description: Qingfeng Zheng et al. performed an approach to utilize ab initio evolutionary algorithm searching for stable compounds in the hafnium-carbon(Hf-C) system.

Materials Project: They reported five titanium carbides in Material Project database.

Qingfeng Zeng, Junhui Peng, Artem R. Oganov, Qiang Zhu, Congwei Xie, Xiaodong Zhang, Dong Dong, Litong Zhang, and Laifei Cheng (2013). Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B 88(21). doi:10.1103/physrevb.88.214107

Citied by 34

(3) Optical quantum confinement in low dimensional hematite†

Description: Mattis Fondell et al. studied the quantum limitations of hematite, a material utilizing in photoelectrochemical cells for solar hydrogen production.

Materials Project: They calculated band diagram for hematite illustrating the direct and indirect transition obtaining data from Materials Project.

Mattis Fondell, T. Jesper Jacobsson, Mats Boman, and Tomas Edvinsson (2014). Optical quantum confinement in low dimensional hematite. J. Mater. Chem. A 2(10). doi:10.1039/c3ta14846g

Citied by 33

(4) High-throughput screening of perovskite alloys for piezoelectric performance and thermodynamic stability

Description: R. Armiento et al. screened a lot of perovskite alloy to exam the optimal properties to accommodate a morphotropic phase boundary, a crucial feature for high piezoelectric performance, in their composition-temperature phase diagram.

Materials Project: They found the stable phase of PZ in the materials project database.

Armiento, B. Kozinsky, G. Hautier, M. Fornari, and G. Ceder (2014). High-throughput screening of perovskite alloys for piezoelectric performance and thermodynamic stability. Physical Review B 89(13). doi:10.1103/physrevb.89.134103

Citied by 30

(5) Learning atoms for materials discovery

Description: Quan zhou et al. showed their work, unsupervised machines, which can learn the basic properties of atoms by themselves from the extensive database of known compounds and materials.

Materials Project: In the data processing step, they inputted all inorganic compounds from Materials Project database.

Quan Zhou, Peizhe Tang, Shenxiu Liu, Jinbo Pan, Qimin Yan, and Shou-Cheng Zhang (2018). Learning atoms for materials discovery. Proceedings of the National Academy of Sciences 115(28). doi:10.1073/pnas.1801181115

Cited by 17

(6) Machine Learning Directed Search for Ultraincompressible, Superhard Materials

Description: Aria Mansouri Tehrani et al. applied a machine learning model to direct related to the synthetic efforts by predicting the elastic moduli. They used support vector machine regression to determine

the highest bulk and shear moduli. Then, they used high-pressure diamond anvil cell measurements to test the machine learning prediction results of bulk modulus which has less than 10% error.

Materials Project: They used crystal structure database which embed in Materials Project.

Aria Mansouri Tehrani, Anton O. Oliynyk, Marcus Parry, Zeshan Rizvi, Samantha Couper, Feng Lin, Lowell Miyagi, Taylor D. Sparks, and Jakoah Brgoch (2018). Machine Learning Directed Search for Ultraincompressible, Superhard Materials. Journal of the American Chemical Society. doi:10.1021/jacs.8b02717

Citied by 14

(7) Do cement nanoparticles exist in space?

Description: G. Bilalbegovi´c et al. put effort in detection of cosmic cement utilizing infrared spectra which calculated from quantum density functional theory.

Materials Project: They used material project to find calcium silicate hydrate.

G. Bilalbegovi, A. Maksimovi, and V. Mohaek-Groev (2014). Do cement nanoparticles exist in space?. Monthly Notices of the Royal Astronomical Society 442(2). doi:10.1093/mnras/stu869

Citied by 4

(8) Ab Initio Investigation of Bi-Rich Bi1–xSbx Alloys

Description: A.R. Khabibulin et al. leveraged ab initio simulation to investigate the atomic and electronic structures of Bi-rich $Bi_{1-x}Sb_x$

Materials Project: Author used Materials Project to generate the supercells which has a different concentrations of Sb element.

A. R. Khabibullin and L. M. Woods (2014). Ab Initio Investigation of Bi-Rich Bi1-xSbx Alloys. Journal of Electronic Materials 43(9). doi:10.1007/s11664-014-3276-1

Citied by 1

(9) Materials informatics for dielectric materials

Description: Yuji Umeda et al. reported an approach for searching new dielectectic materials suitable for use in ceramic capacitors at high frequencies and temperature by a large set of first-principles calculations.

Materials Project: They utilized 3382 candidate compounds from Materials Project database.

Yuji Umeda, Hiroyuki Hayashi, Hiroki Moriwake, and Isao Tanaka (2018). Materials informatics for dielectric materials. Japanese Journal of Applied Physics 57(11S). doi:10.7567/jjap.57.11ub01