Organic Quantum Matter and the Organic Materials Database

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https://omdb.mathub.io

NORDITA

Acknowledgements

current OMDB team

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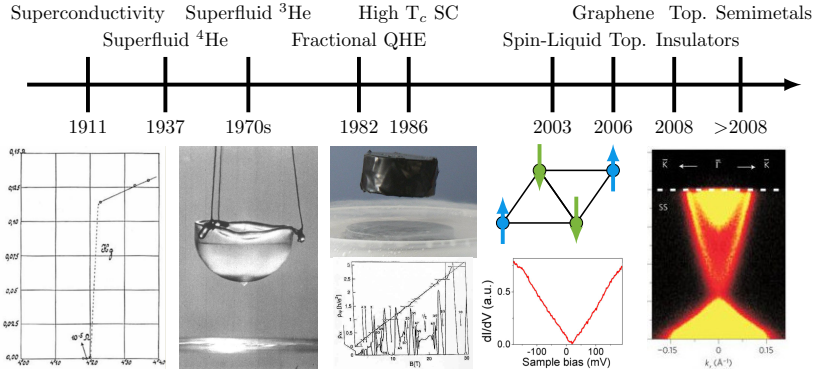
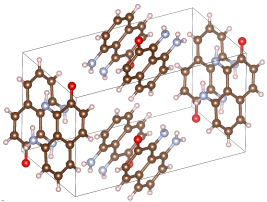
Quantum Materials

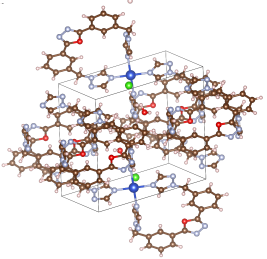
Materials where quantum effects are dominant over a wide range of energy and length scales.

Time line



Organic Materials - Organic Molecular Crystals



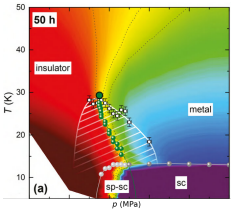


Properties

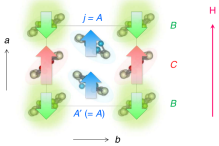
- strong correlations and electron interactions
  $\rightarrow$ complex phase diagrams
- softness $\rightarrow$ flexitronic
- infinite coordination space

Applications

- OLEDs, molecular qubits, spintronics, magnon spintronics, spin liquid physics, ...



E. Gati *et al.*, *Crystals*, **8**(1), 38, (2018)



M. Hirata *et al.*, *Nat. Com.*, **7**, 12666 (2016)

The Organic Materials Database - OMDB

Free to use!

`https://omdb.mathub.io`

S.S. Borysov, RMG, A.V. Balatsky,PloS one, 12:2, 2017

Electronic Structure

- Band structure, DOS

First dataset

- VASP, PBE
- $\approx 25,000$ materials

Second dataset

- VASP, SCAN+VdW (DFT-TS)
- in progress

Magnetic Structure

- Magnon spectra
- Magnetic ground state

First dataset

- RSPT
- linear spin-wave theory
- in progress

Johan Hellsvik, Tue 3 pm

OMDB Community

1. provide/request services
   - synthesis, theory, measurements
2. upload your own results
   - online editorial system
   - reference to your paper
3. "Follow" materials

The Organic Materials Database - OMDB

Workflow

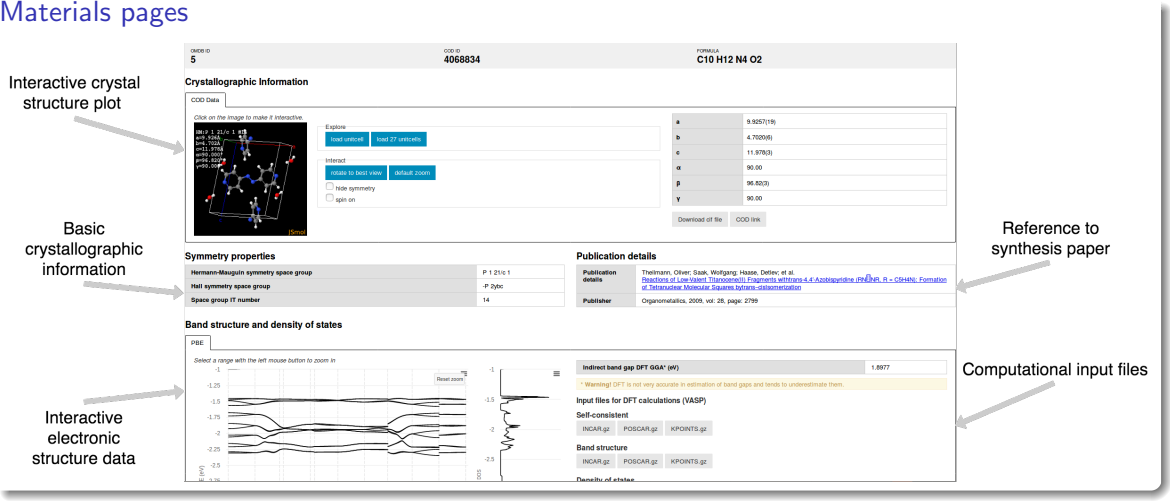
Crystal information
cif-files

Create DFT input files

band structure, DOS
mag. moments, charges
el. properties

The Organic Materials Database - OMDB

Materials pages



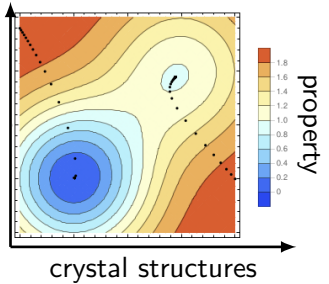
Machine Learning on the OMDB

Machine Learning

- defines a regression (approximate map) between crystal and property

$$f(\text{crystal}) \approx \text{property}$$

- the map is differentiable and allows for minimization tasks

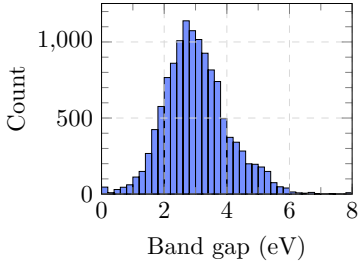


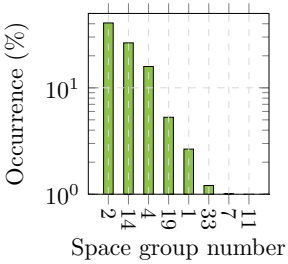
Machine Learning on the OMDB

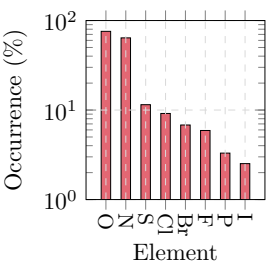
New band gap dataset OMDB-GAP1

B. Olsthoorn, R. M. Geilhufe, S. S. Borysov, A. V. Balatsky, *Adv. Quantum Technol.*, 1900023, (2019)

- band gaps of 12.500 organic molecular crystals
- average 86 atoms in unit cell
- subset of nonmagnetic materials in OMDB
- download at: `https://omdb.mathub.io/dataset`





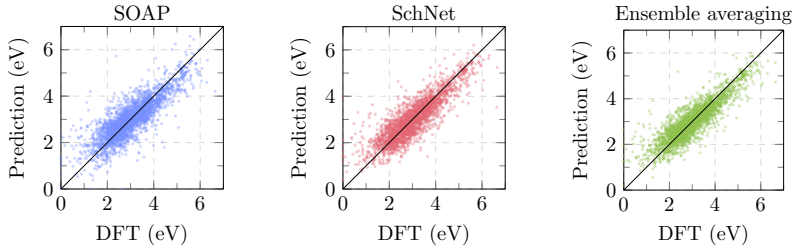


Machine Learning on the OMDB

Benchmark for OMDB-GAP1

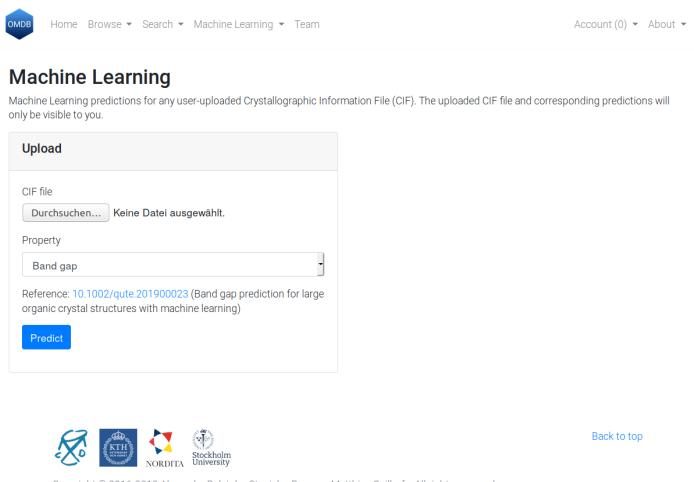
B. Olsthoorn, R. M. Geilhufe, S. S. Borysov, A. V. Balatsky, *Adv. Quantum Technol.*, 1900023, (2019)

- Kernel ridge regression with the SOAP kernel ($n = 8,\ l = 6,\ r_c = 4$Å)
  A. P. Bartók, R. Kondor, G. Csányi, *Phys. Rev. B*, 87, 184115 (2013).
- Deep learning model SchNet ($F = 64,\ T = 3,\ r_c = 5$Å)
  K. T. Schütt, *et al.*, *J. Chem. Phys.*, 148, 241722 (2018).
- best performance MAE 0.361 (eV) for ensemble averaging



Machine Learning on the OMDB

B. Olsthoorn, R. M. Geilhufe, S. S. Borysov, A. V. Balatsky, *Adv. Quantum Technol.*, 1900023, (2019)

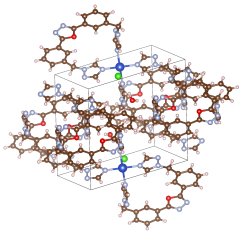


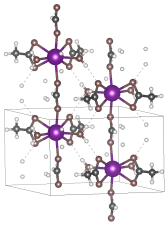
Machine Learning on the OMDB

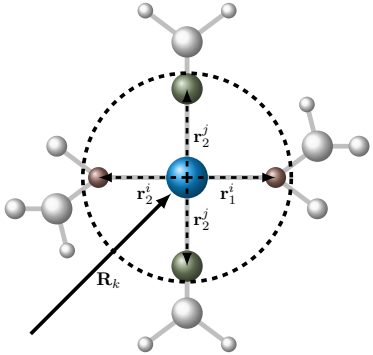
Learning local properties

R. Díaz Perez, RMG, J. Hellsvik, A. V. Balatsky, *in progress*;

- strongly localized properties in organics: mag. moments, charges, etc.
- magnetization of $\approx 200,000$ sites in OMDB crystals
- representation: $\boldsymbol{\nu}^{\text{site}} = [\boldsymbol{\nu}^{\text{OneHot}}, \boldsymbol{\nu}^{\text{Distance}}]$







k^{th} pos.

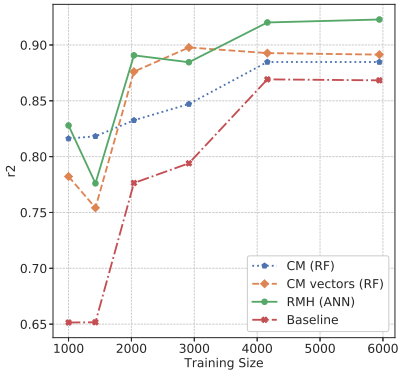
$$\mathbf{v}^{\text{OneHot}} = (0, 0, \ldots, 1, \ldots, 0)$$

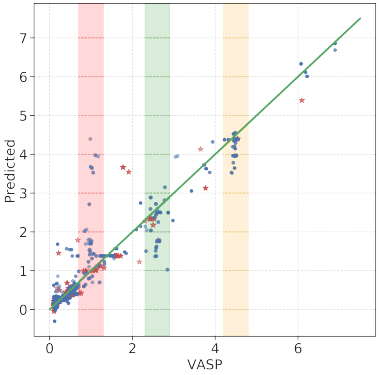
$$\mathbf{v}^{\text{Distance}} = \left(0, \sum_l \frac{1}{|\mathbf{r}_l^i|}, 0, \ldots, \sum_l \frac{1}{|\mathbf{r}_l^j|}, \ldots, 0\right)$$

i^{th} pos. j^{th} pos.

Machine Learning on the OMDB

local properties: site magnetization

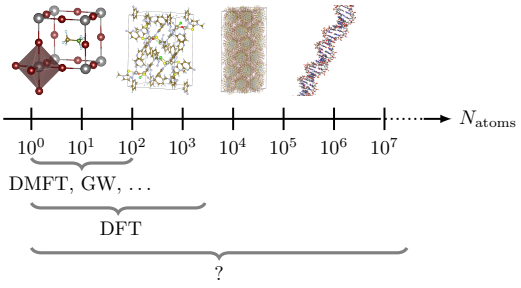




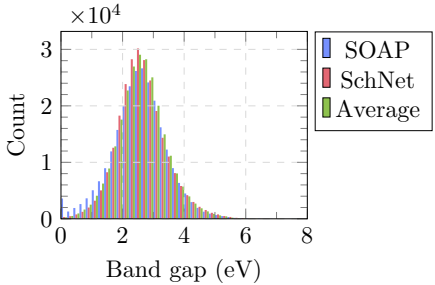
$$r^2 = 1 - \frac{\mathrm{MSE}}{\mathrm{VAR}}$$

Two future outcomes

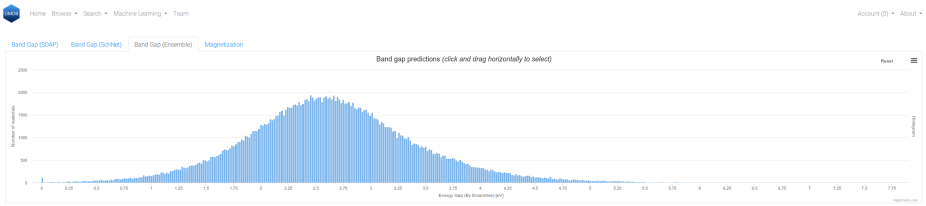
ab initio description of complex materials



Second generation databases



Second generation databases



This is an admin only feature, please don't use it with too many materials

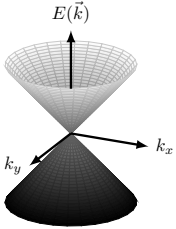
Get zips

199934 results

ID (OMDB)	ID (COD)	Formula	Space group H-M	Space group IT	Publication details	Publisher
1	4082354	$C_{21}\ H_{24}\ Cl_3\ Fe\ N_2$	P -1	2	Dinuclear Iron(0) Complexes of N-Heterocyclic Carbenes	Organometallics, 2014, vol: 33, page: 921
2	4062611	$C_{22}\ H_{24}\ O_2\ Si_2$	P 1 21/c 1	14	2,3,5,6-Tetrasilyl- and 2,3,5,6-tetragermyl-1,4-benzoquinones: X-ray Crystallographic Analysis and DFT Calculations	Organometallics, 2004
3	4077304	$C_{12}\ H_{16}\ Si$	P -1	2	An Effective and Selective Route to 1,5-Dihydropolyalkyletedo-Indacenes: Characterization of Their Mono- and Dianions by Silylation. Structure oftrans-1,5-Bis(trimethylsilyl)-2,6-diethyl-4,8-dimethyl-s-indacene	Organometallics, 2001, vol: 20, page: 5591
4	4070813	$C_{18}\ H_{34}\ Cl_2\ N_4\ P_2\ Si_6$	P -1	2	Titanocene-Mediated Formation of Phosphorus−Phosphorus Bonds	Organometallics, 2008, vol: 27, page: 1393
5	4068834	$C_{10}\ H_{12}\ N_4\ O_2$	P 1 21/c 1	14	Reactions of Low-Valent Titanocene(II) Fragments withtrans-4,4′-Azobispyridine (RN=NR, R = C5H4N). Formation of Tetranuclear Molecular Squares bytrans−cisIsomerization	Organometallics, 2009, vol: 28, page: 2799
6	4072877	$C_4\ H_{15}\ B\ N_6$	P -1	2	Structure and Properties of Substituted Imidazolium, Triazolium, and Tetrazolium Poly(1,2,4-triazolyl)borate Salts	Organometallics, 2007, vol: 26, page: 1782
7	4082978	$C_{22}\ H_{22}\ Br_2\ Cu_2\ N_6$	P -1	2	Remarkable Stability of Copper(I)−N-Heterocyclic Carbene Complexes Void of an Anionic Tether	Organometallics, 2014, vol: 33, page: 2027
8	4073831	$C_{15}\ H_{20}\ F_4\ O_6$	P -1	2	Metal-Dependent Reactivity of Electrophilic Platinum Group Metal Lewis Acid Catalysts: Competitive Alkene Dimerization, Intramolecular Friedel−Crafts Alkylation, and Carbonyl-Ene Reactivity	Organometallics, 2007, vol: 26, page: 5961
9	4069356	$C_{14}\ H_{16}\ N_2\ O_8\ Pt$	P -1	2	Mono(2,6-dinitroaryl)platinum(II) and Mono- and Bis(2,6-dinitroaryl)platinum(IV) Complexes	Organometallics, 2009, vol: 28, page:

Applications of the OMDB - (Organic) Dirac-materials

Dirac materials



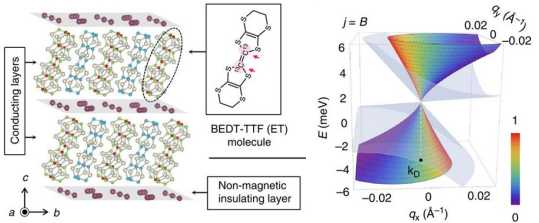
- excitations effectively behave as Dirac particles
  T. Wehling, et al., Adv. Phys., 63:1, 2014

$$E^{\pm}(\boldsymbol{k}) = \pm\sqrt{\hbar^2\boldsymbol{k}^2 + m^2 v_D^4}$$

- graphene
- Dirac and Weyl semimetals
- topological insulators

Organic Dirac materials

- 2-dimensional organic frameworks
  L. Wei *et al.*, *Phys. Chem. Chem. Phys.*, **18**, (2016)
  M. Wu *et al.*, *2D Materials*, **4**, 015015 (2017)
- (BEDT-TTF)-based charge transfer salts (under pressure $\approx$ 2.3 GPa)



M. Hirata *et al.*, *Nat. Com.*, **7**, 12666 (2016)

Mine for Patterns in the OMDB

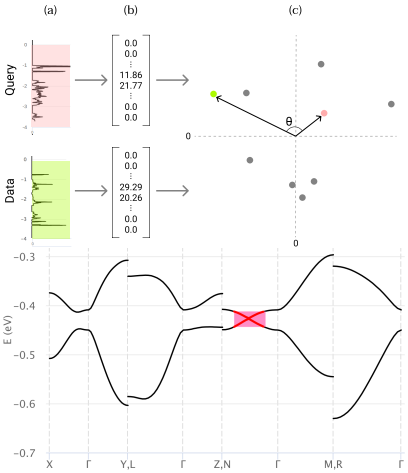
RMG, S. S. Borysov, D. Kalpakchi, & A. V. Balatsky, *Phys. Rev. Mat.* 2, 024802 (2018)
S. S. Borysov, B. Olsthoorn, M. B. Gedik, RMG, A. V. Balatsky, *npj Computational Materials* **4**, 46 (2018)

Similarity search

- represent electronic structure (DOS, bands) as highly dimensional vectors
- search for similarities of a pattern via vector distance, e.g.

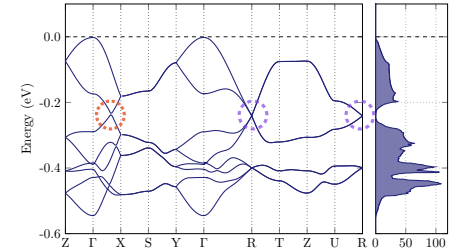
$$d = \sqrt{2 - 2\cos\theta}$$

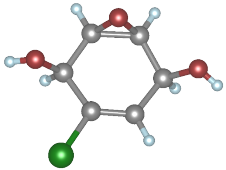
- Ball Tree nearest neighbor search

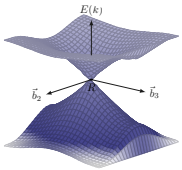


Topological nodes in organic materials

Point nodes

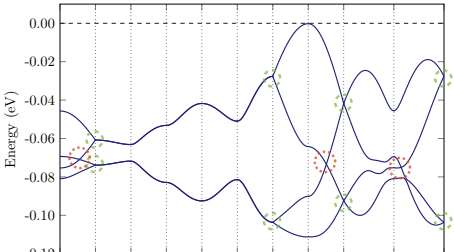


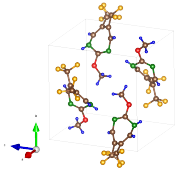


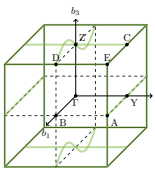


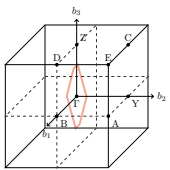
RMG, *et al.*, *Sci. Rep*, **7**, 7298 (2017)

Line nodes









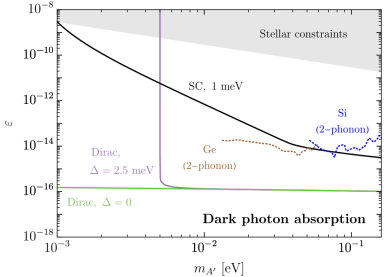
RMG, *et al.*, *Phys. Rev. B*, **95**, 041103(R) (2017)

Further examples: Dirac Materials for Dark Matter sensors

DM for DM

- search for sub-GeV dark matter (DM)
- coupling ord. photon to dark photon

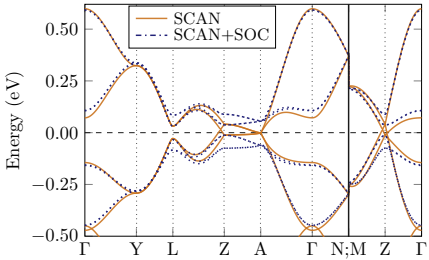
$$\mathcal{L}_{\text{coupling}} = -\frac{\epsilon}{2} F^{\mu\nu} F'_{\mu\nu}$$



Y. Hochberg, *et al.*, *Phys. Lett. B*, **772** (2017)
Y. Hochberg, *et al.*, *PRD*, **97**.1, 015004 (2018)

Mining for materials candidates

- escape vel. v_{max} for DM bound to halo
- $v_D < v_{\text{max}} \approx 600\text{km s}^{-1}$
- tiny gap required $\rightarrow$ tiny SOC in organics
- (BEDT-TTF)·Br



RMG, *et al.*, *PSS RRL*, **12**, 1800293 (2018)
M. Winkler, F. Kahlhoefer, RMG, *et al.*, *in prep.*

Further examples: Towards high-T_c organic superconductors

Online Density of States Similarity Search Tool

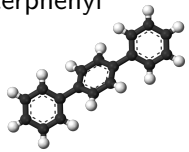
R.M. Geilhufe, *et al.*, *Phys. Rev. Mat.* 2, 024802 (2018)

- upload DOS of a reference material
- obtain results for similar materials

Example: high-temperature superconductors

Reference material

p-terphenyl



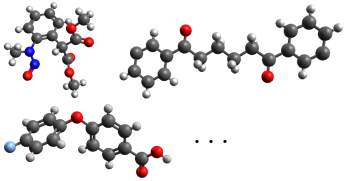
Transition temperature 123 K

R.-S Wang, *et al.*, *arXiv:1703:06641 (2017)*

OMDB

Mining results

15 novel high-T_c candidates



R.M. Geilhufe, *et al.*, *Phys. Rev. Mat.* 2, 024802 (2018)

Summary

Organic Materials Database

- Free to use!

  `https://omdb.mathub.io`

- currently $\approx 25,000$ materials stored
- contains non-trivial search functionality (pattern matching)
  S. S. Borysov, B. Olsthoorn, M. B. Gedik, RMG, A. V. Balatsky, *npj Computational Materials* **4**, 46 (2018)
- OMDB-Gap1 dataset, machine learning for band gap prediction
  B. Olsthoorn, RMG, S. S. Borysov, A. V. Balatsky, *arXiv:1810.12814*
- second generation databases
- data-mining + symmetry analysis organic semimetals
  RMG, *et al.*, *Sci. Rep*, **7**, 7298 (2017)
  RMG, *et al.*, *Phys. Rev. B*, **95**, 041103(R) (2017)