

Supporting Information for

Reducing Time to Discovery: Materials and Molecular Modeling, Imaging, Informatics and Integration

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M3I3 Related Initiatives



Figure S1. Photography of KAIST 2031 Vision Day in 2018. M3I3 logo design by Hosun Jun. Reprinted with permission from Hosun Jun (creator of M3I3 logo) and Seungbum Hong (person in the picture).

1. USA, Materials Genome Initiative (MGI) [mgi.gov]

- To create an era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost.
- Activities
 - Integration of Experiments, Computation and Theory
 - Facilitate Access to Materials Data
 - Equip the Next-Generation Materials Workforce
 - Enable a Paradigm Shift in Materials Development
- **Centers:**

- CHiMaD (Northwestern Univ.) [<http://chimad.northwestern.edu/>]
- JCESR (Argonne National Lab.) [<http://www.jcesr.org/>]
- PRISMS (University of Michigan) [<http://www.prisms-center.org/>]
- Multidisciplinary University Research Initiative: Managing the Mosaic of Microstructure [<http://muri.materials.cmu.edu/>]
- CEIMM [<http://ceimm.jhu.edu/>]

- **Database Platforms (Data Generation, Curation and Repository)**
 - Materials Project [<https://www.materialsproject.org/>]
 - Materials Data Facility [<https://materialsdatafacility.org/>]
 - OQMD [<http://oqmd.org/>]
 - NIST MD Repository [<https://materialsdata.nist.gov/>]
 - PFHub: The Phase Field Community Hub [<https://pages.nist.gov/pfhub/>]
 - JARVIS (JARVIS-DFT, JARVIS-FF, JARVIS-ML) [<https://jarvis.nist.gov/>]
 - AFLOW [<http://www.aflowlib.org>]
 - Materials Commons (<https://materialscommons.org/>)
 - Polymer Property Predictor and Database [<https://pppdb.uchicago.edu/>]
 - Materials Resource Registry [<https://materials.registry.nist.gov/>]

2. EU, Novel Materials Discovery (NOMAD) [<https://nomad-coe.eu/>]

- To establish the fourth paradigm in computational materials science with the recognition that big data contain correlations, reflected in terms of structure and patterns in the data that are not visible in small data sets.
- To draw “materials maps” that allow us to find materials that are useful for a particular application in the structural and chemical compound space.
- **Centers:**
 - NOMAD Lab [<https://nomad-lab.eu/>]
 - FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids [<https://www.fair-di.eu/fairmat/consortium>]
- **Database Platforms (Data Generation, Curation and Repository)**
 - FAIR-DI [<https://www.fairdi.eu/>]
 - NOMAD Repository and Archive [<https://nomad-lab.eu/prod/rae/gui/search>]
 - NOMAD Encyclopedia [<http://nomad-lab.eu/prod/rae/encyclopedia/#/search>]
 - NOMAD AI Toolkits [<https://analytics-toolkit.nomad-coe.eu/hub>]

3. Switzerland, Materials Revolution: Computational Design and Discovery of Novel Materials (MARVEL) [<https://nccr-marvel.ch/>]

- The accelerated design and discovery of ~~new~~ novel materials, *via* a materials’ informatics platform of database-driven high-throughput quantum simulations, powered by

- advanced electronic-structure capabilities, for predictive accuracy
- innovative sampling methods to explore configuration/composition space
- application of big-data concepts to computational materials science
- **Centers:**
 - The NCCR MARVEL [<https://nccr-marvel.ch/project>]
- **Database Platforms (Data Generation, Curation and Repository)**
 - AiiDa [<http://www.aiida.net/>]
 - Materials Cloud [<https://www.materialscloud.org/>] (A platform for open science with educational, research, and archiving tools, simulation software and services, curated and raw data)
 - Quantum Mobile [<https://quantum-mobile.readthedocs.io/en/latest/>]

4. Japan, MI²I: Materials research by Information-Integration Initiative [<https://www.nims.go.jp/MII-I/en/>]

- To create an open innovation hub for data-driven (information-integrated) materials research, so called “materials informatics”
- **Centers:**
 - The Center for Materials research by Information Integration (CMI²)
- **Database Platforms (Data Generation, Curation and Repository)**
 - MI²I data platform [<https://www.nims.go.jp/MII-I/en/MI2I-DPF.html>]
 - The NIMS Materials Database (MatNavi) [<https://mits.nims.go.jp/en/>] (Polymer DB (chemical structures, polymerization, processing, physical properties, NMR

spectra, *etc.*), Inorganic MaterialDB (crystal structures, phase diagrams, physical properties, *etc.*), Metallic Material DB (density, elastic constants, creep characteristics, *etc.*) and Computational Electronic Structure DB (band structures obtained by first-principles calculations, *etc.*). It also offers applications such as the Composite Design & Property Prediction System).

- AtomWork-Adv [<https://atomwork-adv.nims.go.jp/en/service.html>] (a database that contains data on the crystal structure, X-ray diffraction, properties, and state diagrams of inorganic materials extracted from scientific literature)

5. China, Materials Genome Engineering (MGE) project

- Database and Big Data Technology of Material Genome Engineering (MGE)
- Data acquisition and database fusion technology on structure -property based on high-throughput experiments and calculations
- **Centers:**
 - Material Genome Engineering Database and Big Data Technology
- **Database Platforms (Data Generation, Curation and Repository)**
 - Materials Scientific Data Sharing Network [www.materdata.cn]
 - National Environmental Corrosion Platform

6. Korea, KAIST M3I3 and Data-based Materials Research Innovation

- To create an innovation hub for integrating materials research data and accelerate the full cycle of materials research and development.
- **Centers:**
 - KAIST [<https://www.kaist.ac.kr/en/html/research/04.html>]
 - KRISS [<https://www.kriss.re.kr/eng/main/main.html>]

- KISIT [<https://www.kisti.re.kr/>]

Database Platforms (Data Generation, Curation and Repository)

- Materials Research Data Platform
- Materials Square Education [<https://edu.materialssquare.com/>]

Table S1. Summary of M3I3 related initiatives in the world.

Initiative	Centers	Database Platforms
MGI (USA)	CHiMaD, JCESR, PRISMS, MURI, CEIMM, <i>etc.</i>	Materials Project, MDF, OQMD, NIST MD, PFHub, JARVIS, AFLOW, Materials Commons, PPPD, MRR
NOMAD (EU)	NOMAD Lab, FAIR-DI for CMP and CPS	FAIR-DI, NOMAD Repository and Archive, NOMAD Encyclopedia, NOMAD AI Toolkits
MARVEL (CH)	The NCCR MARVEL	AiiDa, Materials Cloud, Quantum Mobile
MI ² I (Japan)	CMI ²	MI2I data platform, MatNavi, AtomWork-Adv
MGE (China)	MGE Database and Big Data Technology	Materials Scientific Data Sharing Network, National Environmental Corrosion Platform
M3I3, MRI (Korea)	KAIST, KRISS, KISTI	Materials Research Data Platform

Table S2. Selected and curated data from ref 111 in the main text for Li-rich electrodes.

Li	Ni	Co	Mn	O	sin_temp	sin_t	cut_off	c_rate	m_temp	prim_size	sec_size	Dis_cap	sum(Li : Mn)	sum(Ni: Mn)
1.31	0.02	0.02	0.65	2	900	10	4.8	0.05	nan	0.17	6.71	184	2	0.69
1.27	0.05	0.05	0.63	2	900	10	4.8	0.05	nan	0.17	10.78	195	2	0.73
1.2	0.1	0.1	0.6	2	900	10	4.8	0.05	nan	0.13	10.3	268	2	0.8
1.11	0.17	0.17	0.55	2	900	10	4.8	0.05	nan	0.32	19.57	249	2	0.89
1.05	0.21	0.21	0.53	2	900	10	4.8	0.05	nan	0.3	22.68	230	2	0.95
1.2	0.15	0.1	0.55	2	900	6	4.8	0.1	25	nan	nan	236.1	2	0.8
1.2	0.15	0.1	0.55	2	900	6	4.8	0.1	55	nan	nan	296.2	2	0.8
1.2	0.17	0.16	0.47	2	950	10	4.8	0.077	25	nan	nan	195.1	2	0.8
1.2	0.13	0.13	0.54	2	850	20	4.8	0.1	nan	0.195	3.3	289.7	2	0.8
1.2	0.13	0.13	0.54	2	850	20	4.8	0.1	nan	0.172	2.4	267.5	2	0.8
1.2	0.12	0.12	0.56	2	900	12	4.8	0.5	22	0.2	1	236.7	2	0.8
1.2	0.12	0.12	0.56	2	900	12	4.8	0.5	22	0.15	1.2	264.6	2	0.8
1.2	0.12	0.12	0.56	2	900	12	4.8	0.5	22	0.3	nan	209.8	2	0.8
1.2	0.12	0.12	0.56	2	900	12	4.8	0.5	22	1	nan	156.3	2	0.8
1.2	0.16	0.08	0.56	2	800	15	4.8	0.1	40	0.0425	1.25	296	2	0.8
1.2	0.1	0.1	0.6	2	800	8	5	0.2	nan	0.06	5.5	242	2	0.8
1.2	0.13	0.13	0.54	2	800	10	4.8	0.1	25	0.05	1	309.9	2	0.8
1.2	0.175	0.1	0.525	2	nan	nan	4.9	0.2	25	nan	nan	260	2	0.8
1.2	0.17	0.07	0.56	2	900	12	4.8	0.1	nan	0.5	nan	201	2	0.8
1.144	0.136	0.136	0.544	2	850	15	4.6	0.1	20	0.15	nan	292.1	1.96	0.816
1.144	0.136	0.136	0.544	2	850	15	4.6	0.1	30	0.15	nan	259.9	1.96	0.816
1.144	0.136	0.136	0.544	2	850	15	4.6	0.1	20	0.15	nan	221.4	1.96	0.816
1.16	0.12	0.12	0.6	2	900	12	4.8	0.2	30	0.29	nan	278	2	0.84
1.16	0.12	0.12	0.6	2	650	24	4.8	0.2	30	0.32	nan	302	2	0.84
1.2	0.12	0.12	0.56	2	900	12	4.8	0.5	25	0.22	nan	258.3	2	0.8
1.17	0.17	0.1	0.56	2	850	12	4.6	0.05	25	nan	17.2	253.9	2	0.83
1.23	0.09	0.12	0.56	2	nan	nan	4.8	0.1	25	0.19	nan	250.8	2	0.77
1.2	0.17	0.16	0.47	2	950	10	4.8	0.06	25	nan	nan	195	2	0.8
1.2	0.175	0.1	0.525	2	nan	nan	nan	nan	nan	nan	nan	nan	2	0.8
1.2	0.13	0.13	0.54	2	950	12	4.8	0.05	nan	0.35	nan	257.43	2	0.8
1.2	0.2	0	0.6	2	nan	nan	4.8	0.1	nan	nan	nan	nan	2	0.8
1.2	0.17	0.07	0.56	2	900	12	4.8	0.08	nan	nan	nan	291	2	0.8
1.17	0.25	0	0.58	2	850	10	4.8	0.1	nan	nan	nan	260.8	2	0.83
1.2	0.15	0.1	0.55	2	nan	nan	4.8	0.084	nan	nan	nan	252	2	0.8
1.2	0.13	0.13	0.54	2	nan	nan	4.8	0.05	nan	0.3	nan	279	2	0.8

In the main text, most processes in the M3I3 are explained based on inorganic crystal materials. However, the basic principle will be the same for molecules in the battery system. For example, in the case of PVDF, which is the well-known binder for the Li ion battery, there are five crystalline polymorphs, namely, α -, β -, γ -, δ -, and ε -phases, which depend upon the CH_2/CF_2 dipole arrangements.¹

From the molecule point of view, the basic unit will be as shown in Figure S2 for all five polymorphs, where two carbons are connected to each other and two hydrogens and two fluorine atoms *via* covalent bonding.²

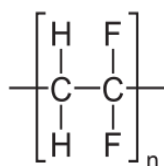


Figure S2. The general molecular structure of PVDF. Reprinted from reference 2 with permission. This structural formula is ineligible for a copyright and therefore in the public domain.

This unit will arrange in a polymer chain with different conformations depending on the processing route as shown in Figure R4, but usually will from alpha phase.^{3,4}

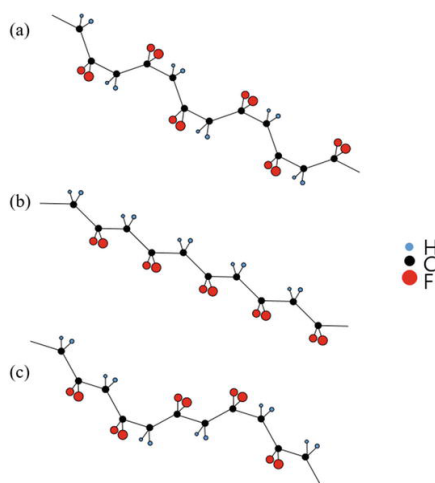


Figure S3. Configuration in the unit cell of (a) the α -phase, (b) the β -phase, and (c) the γ -phase. Reprinted under a Creative Commons Attribution 3.0 License from reference 3 with permission. Copyright 2019 Jeongjae Ryu, Seongmun Eom, Panpan Li, Chi Hao Liow and Seungbum Hong.

As we scale up to the micron scale (grain and grain boundaries), one can start to characterize the materials using XRD, FTIR and SEM images.⁴ XRD characterizes the unit cell or molecular chain crystal structure, FTIR characterizes the molecular structure and its bending motion, and SEM visualizes the grain and grain boundary or porosity in the microstructure. The structure at each scale such as PVDF molecule, molecular chain and grain/grain boundary/pore will influence the dipole moment at atomic scale, piezoresponse at nanoscale, and polarization at micron scale as shown in Fig. S4. As such, the multiscale structure-property relationship of PVDF can be depicted as in Fig. S4.^{5,6}

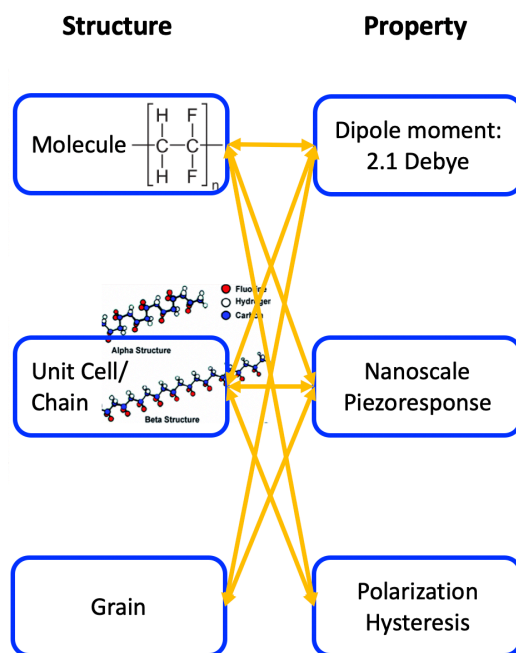


Figure S4. The multiscale structure-property relationship of PVDF. Adapted under a Creative Commons Attribution 3.0 License from references 2 and 3 with permission. Copyright 2019 Jeongjae Ryu, Seongmun Eom, Panpan Li, Chi Hao Liow and Seungbum Hong.

Regarding the processing-structure relationship, one example is shown in Fig. S5, where the applied electric field and the addition of cold drawing or annealing under high pressure will be the input of processing and the output structure could be alpha, delta or beta phase depending on the input parameters.⁷

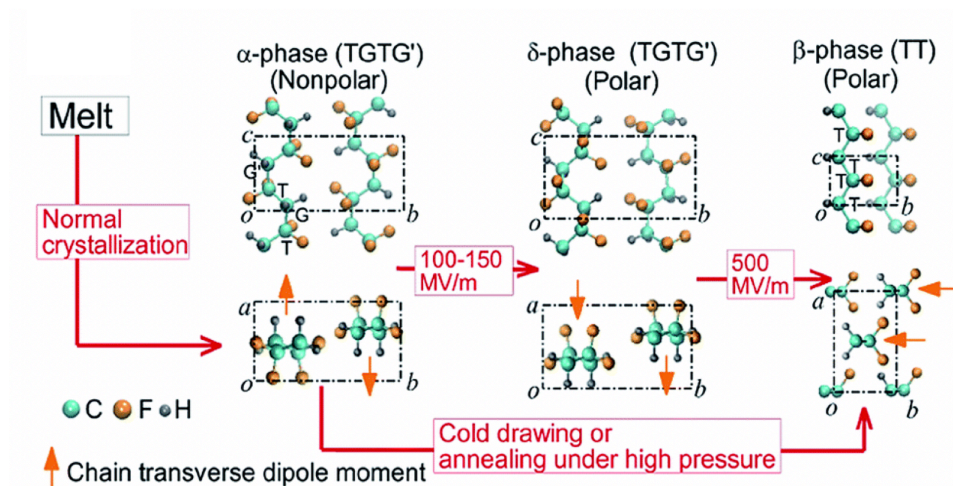


Figure S5. The processing steps of PVDF from melt. With application of electric field and addition of cold drawing step or annealing under high pressure, one can get different crystal structures. Reprinted with permission from reference 7. Copyright© American Institute of Physics 2016.

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