

# Discovery of MOFs for Hydrogen Storage via Machine Learning and First Principles Methods

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## ABSTRACT

Hydrogen energy provides an approach to addressing the energy crisis and global climate change. However, additional energy consumption and carbon emission in the conventional storage process of H<sub>2</sub> tackle the hydrogen economy's prosperity. Metal-organic frameworks (MOFs), new type materials with exciting structures and properties, represent a blueprint for realizing large-scale applications of hydrogen energy by lowering energy consumption and cost of facilities. Traditional hydrogen storage MOFs have stepped to an advanced level, and the discovery inevitably slows down. Materials are fundamental to low-cost hydrogen storage, and the screening and design of H<sub>2</sub> storage MOFs are crucial for the hydrogen economy. We aim to propose a novel paradigm of hydrogen storage MOFs material design that combines machine learning and first principles calculation, such as density functional theory (DFT). By constructing an active learning framework and using DFT calculation results as training data, a self-improving model that can screen existing material databases and guide experiments design is obtained. The prediction model's performance is examined in conventional ways (root mean square error, coefficient of determination, etc.) and will be further tested in practical considerations (test the performance of MOFs guided by the model).

**Keywords:** hydrogen energy, MOF, machine learning, density functional theory

## NONMENCLATURE

### Abbreviations

AI	Artificial Intelligence
DFT	Density Functional Theory
DNN	Deep Neural Network
HF	Hartree Fock
ML	Machine Learning
MOF	Metal-Organic Framework
RF	Random Forest

## 1. INTRODUCTION

Hydrogen energy, with environmental-friendly chemical reactions and high calorific value, is regarded as the most promising candidate for fossil fuels. However, expensive storage and separation of hydrogen tackle large-scale hydrogen applications. The key to alleviating the cost lies in the novel, high-performance materials. Metal-Organic Frameworks (MOFs) are a type of material with novel structures and interesting properties. Many pioneers have proved MOFs' capability in hydrogen storage [1], but there is still a gap between current performances and application demands. As comparatively simple MOFs have been investigated, MOFs' complexity and high experimental costs slow down the discovery of MOFs for hydrogen storage. Thoroughly Screening the enormous MOFs' design space by conventional research paradigm (i.e., trial and error) is impossible both in time and finance.

Hence, AI (artificial intelligence) for science, an emerging interdisciplinary research paradigm, should be considered. With its inherent capability in analyzing massive high-dimensional data, AI has been a powerful assistant to scientists, especially machine learning (ML). ML accelerated discovery of materials has been a hot topic recently [2]. Nevertheless, debates over the interpretability of ML models, especially deep learning, have not stopped yet, making someone prudent toward pure data-driven methods.

When it comes to matter and chemistry, compared with machine learning models, widely-used theoretical methods are based on solid theory or contain more physics, which makes them more persuasive to material scientists. Meanwhile, booming computation power turns 'ab initio' or first principles calculation of large systems into truth. Among the various methods, density functional theory (DFT) distinguished itself with accuracy near post-Hartree Fock (post-HF) and cost close to Hartree Fock (HF). DFT dominates in the calculation for periodic systems at the electronic structure level and is suitable for MOFs. Among the

three methods mentioned before, experimental methods are the most expensive but most accurate; ML models reach comparatively high accuracy with low cost, while theory calculation methods stand in the middle, shown in Figure 1A. Herein, a three-stage paradigm can be proposed in Figure 1B: ML models screen through the massive MOFs' database (CoRE MOF

[3], about 10k) and pick out the candidates (about 100); DFT calculation predicts the high-performance MOFs through specific parameters (e.g., hydrogen absorption enthalpy); several MOFs are synthesized and test at the last stage. Up to now, we have finished the first stage and believe the output will be satisfied.

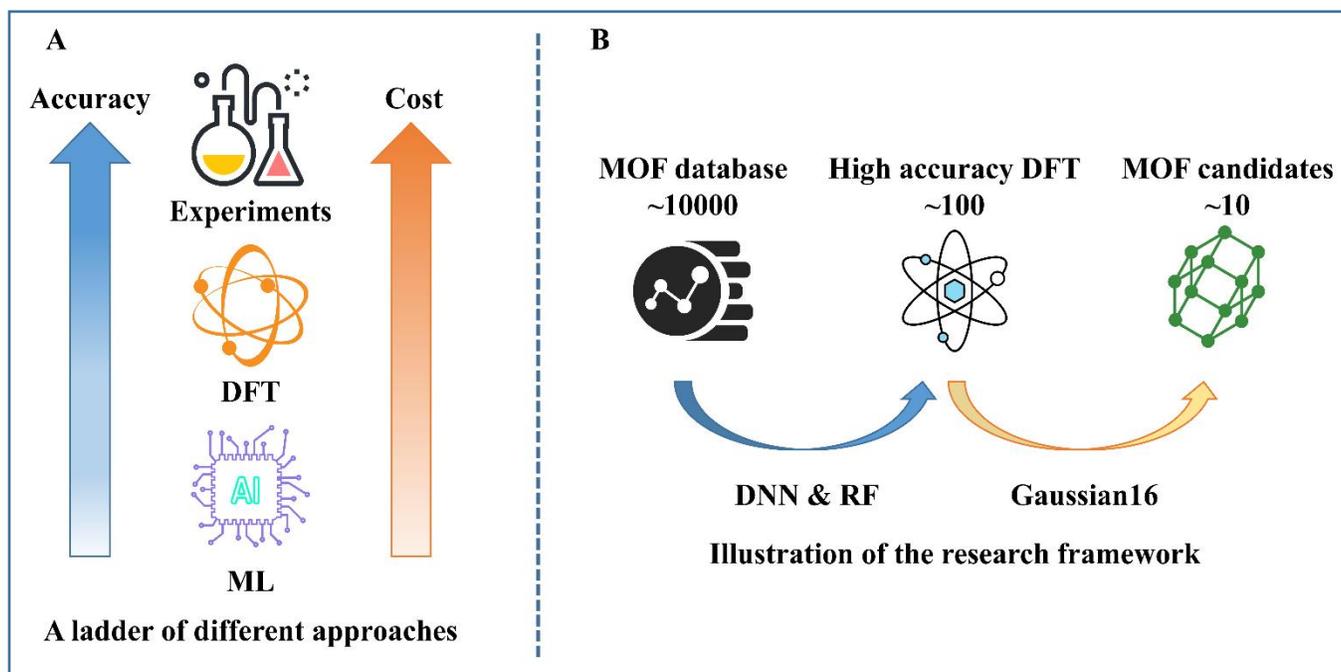


Fig. 1 the logic and framework of this work. A: a comparison of accuracy and cost among three methods. B: an illustration of a three-stage discovery of MOFs for hydrogen storage.

## 2. METHODS

### 2.1 Deep Neural Network (DNN)

DNNs, as a machine learning algorithm, can achieve optimized results by adjusting the weights of each layer. In general, DNNs with more than one hidden layer have been shown to surpass conventional and statistical models in various applications [4]. The application of deep learning to the materials field is attracting more and more attention, while little research has been developed to make suitable predictions for hydrogen adsorption using a data-driven approach via deep learning. In this work, a four hidden layers DNN is trained and applied.

### 2.2 Random Forest (RF)

RF models are a subset of decision trees. Decision tree models are inherently better than 'black-box' models in interpretability because a series of logic tests is contained. A decision tree model use nodes to classify features, and the branches indicate which features are

selected. Too big a decision tree size is prone to overfitting, severely reducing the model's generalizability. RF models [5] use ensemble techniques to prevent overfitting.

### 2.3 Density functional theory (DFT)

DFT is based on the Hohenberg-Kohn theorems, which prove that all the ground state properties of a many-electron system are determined by electron density distribution [6] (i.e., density functionals). By selecting appropriate electron density, the state with minimum energy is the ground state, and corresponding properties are easily attained. Generally, the total energy in DFT contains three parts: kinetic energy, exchange-correlation energy, and classic coulomb potential energy. Limited by the absence of accurate kinetic energy functionals, today's DFT is Kohn-Sham DFT [7], which introduces atomic orbitals into DFT and collects the uncertainty in the exchange-correlation part. For hydrogen storage using MOFs, an empirical model has shown that the optimized enthalpy of

dissociation is about 22-25 kJ/mol [8] under practical conditions. We will use a cluster model (about 200 atoms scale) to describe the combination and dissociation of MOFs and hydrogen. At this scale, double hybrid functionals are incredibly time-consuming, and pure functionals lack enough accuracy. We plan to use the classic functional B3LYP-D3(BJ) [9, 10] and 6-31G\*\* [11] because van der Waals forces are very critical in the combination between MOFs and hydrogen. For MOFs containing heavy atoms, pseudopotential will be applied to specific atoms.

### 3. RESULTS

Our DNN is trained with 137 MOF's data points reported by previous works shown in Table S1 in the Supporting Information, using pore diameter, surface area, pore volume, temperature, and pressure as the input variables, respectively. Then, the DNNs with an implicit relationship between the structural properties and hydrogen adsorption is employed to predict the possible hydrogen adsorption capacities of MOFs.

Meanwhile, we use the RF model to measure the relative importance of input features on the MOFs' hydrogen storage capability. The results show that Brunauer-Emmett-Teller (BET) surface and pore volume are the most critical intrinsic parameters, as Figure 2 shows.

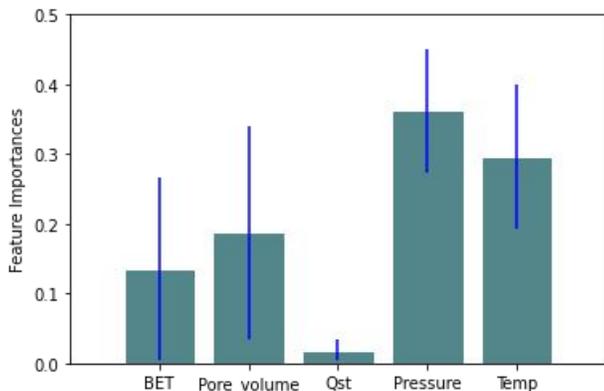


Fig. 2 The relative importance of input features on the hydrogen storage using RF model.

The most critical hyper-parameters in the DNN model, including max iteration during training and learning rate, were constantly adjusted by the grid search method with the  $R^2$  score [12]. The best model with the highest  $R^2$  score was selected. Meanwhile, the RF model was also optimized by adjusting the number of trees ranging from 50 to 500 and the number of features from 1 to 5 with a step size of 1. The hyper-parameters corresponding to the best-performing models were selected and used to validate models with 5-fold cross-validation, respectively. The predicted

outputs in the test groups plotted versus the corresponding experimental values with the two models are shown in Figure 3. The overall MSE values and  $R^2$  score values (0.989) developed by the DNN algorithm show that DNN has high accuracy, and the prediction ability of the DNN model for gas adsorption has been proved in previous studies. On the contrary, the MSE of the RF model was higher than that using the DNN model. Such results demonstrate that DNN is superior to RF in predictive accuracy.

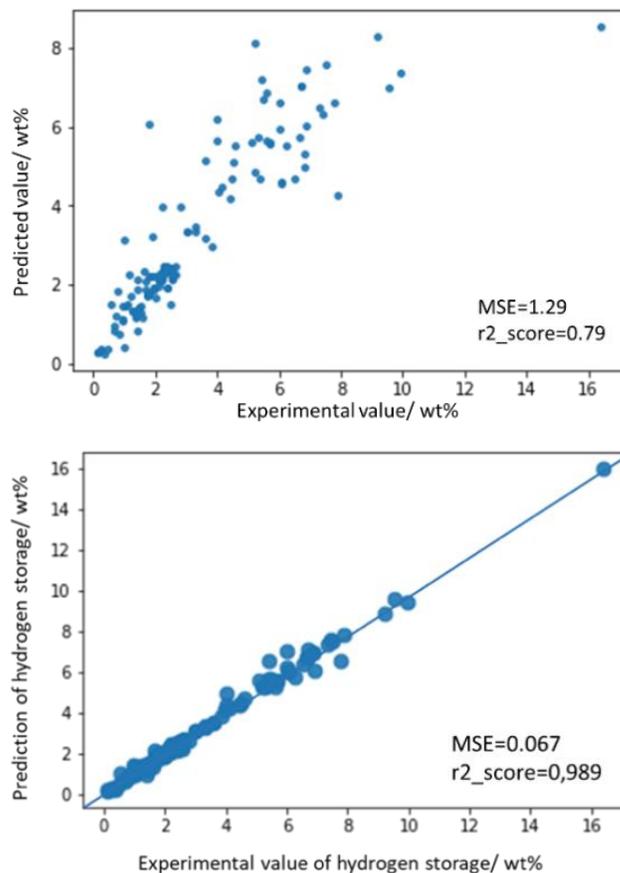


Fig. 3 Comparison of predicted hydrogen storage and experimental data using DNN (right) and RF (left) model with 5-fold cross validation.

### 4. CONCLUSIONS

We proposed a three-stage discovery strategy of MOFs for hydrogen storage, and the first step has been implemented. Nevertheless, there are some drawbacks of current works: limited to experimental costs, data from public literature is far lower than an ideal amount, which may cause overfitting and decrease the ML models' reliability; experimental conditions in hydrogen storage are very complex. Thus, DFT calculation should consider parameters such as solvation effects and ambient temperature (DFT's results are at OK in default). In order to overcome small samples' harm, novel ML methods can be applied, such as active

learning. Other simulation methods, such as molecular dynamics, can also be a powerful tool. Although there is much to improve, we believe this paradigm is rational and correct.

## ACKNOWLEDGEMENT

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## 1. Data collection (1) Tabulated data

Serial Number	BET surface area/(m <sup>2</sup> /g)	pore volume/(cm <sup>3</sup> /g)	Q <sub>st</sub> /(kJ/mol)	Pressure/e/bar	Temp/K	gravimetric hydrogen storage/wt%	Reference
1	1560	0.696	6.63	1	77	2.51	Inorg. Chem. 2011, 50, 5044
2	1560	0.696	6.63	40	77	4.14	Inorg. Chem. 2011, 50, 5044
3	1560	0.696	6.63	100	298	0.46	Inorg. Chem. 2011, 50, 5044 Cryst. Growth Des. 2011, 11, 5064–5071
4	1490	0.605	7.24	1	77	2.36	Inorg. Chem. 2011, 50, 5044
5	2847	1.01	9.5	1	77	2.4	J. Am. Chem. Soc. 2008, 130, 1833
6	1660	0.667	6.56	1	77	2.27	Inorg. Chem. 2011, 50, 5044
7	782	0.39	8.3	1	77	1.77	J. Am. Chem. Soc. 2006, 128, 1304 J. Am. Chem. Soc. 2007, 129, 15740
8	2300	1	7.3	1	77	2.1	J. Am. Chem. Soc. 2007, 129, 15740
9	2300	1	7.3	45	77	5.7	J. Am. Chem. Soc. 2007, 129, 15740 Angew. Chem., Int. Ed. 2006, 45, 7358
10	1670	0.68	6.3	1	77	2.59	Angew. Chem., Int. Ed. 2006, 45, 7358 J. Am. Chem. Soc. 2009
11	1670	0.68	6.3	20	77	4.02	J. Am. Chem. Soc. 2009
12	2247	0.89	5.3	1	77	2.52	Angew. Chem., Int. Ed. 2006, 45, 7358 Angew. Chem., Int. Ed. 2006, 45, 7358
13	2247	0.89	5.3	20	77	6.06	Angew. Chem., Int. Ed. 2006, 45, 7358 J. Am. Chem. Soc. 2009
14	2932	1.14	5.4	1	77	2.24	J. Am. Chem. Soc. 2009
15	2932	1.14	5.4	20	77	6.07	J. Am. Chem. Soc. 2009
16	2929	1.142	5.71	1	77	2.63	J. Am. Chem. Soc. 2009
17	2929	1.142	5.71	20	77	6.51	J. Am. Chem. Soc. 2009
18	2929	1.142	5.71	60	77	7.78	J. Am. Chem. Soc. 2009
19	2387	0.898	5.77	1	77	2.52	J. Am. Chem. Soc. 2009
20	2387	0.898	5.77	20	77	5.4	J. Am. Chem. Soc. 2009
21	1855	0.798	6.34	1	77	2.29	J. Am. Chem. Soc. 2009

22	1855	0.798	6.34	20	77	J. Am. Chem. Soc. 2009 4.5 131, 2159
23	1822	0.767	6.7	1	77	J. Am. Chem. Soc. 2009 2.26 131, 2159
24	1822	0.767	6.7	20	77	J. Am. Chem. Soc. 2009 4.46 131, 2159
25	2960	1.22	5.68	1	77	2.64 Chem.—Eur. J. 2009, 15, 4829
26	2960	1.22	5.68	55	77	5.43 Chem.—Eur. J. 2009, 15, 4829
27	2930	1.19	6.21	1	77	2.56 Chem.—Eur. J. 2009, 15, 4829
28	2930	1.19	6.21	48	77	5.47 Chem.—Eur. J. 2009, 15, 4829
29	1407	0.67	6.8	1	77	2.34 Chem. Mater. 2008, 20, 3145
30	1407	0.67	6.8	3.5	30	6.84 Chem. Mater. 2008, 20, 3145
31	1407	0.67	6.8	45	300	0.25 Chem. Mater. 2008, 20, 3145 Chem.
32	2500	1.012	7.2	1	77	1.95 Commun. 2010, 46, 4196 Chem.
33	2500	1.012	7.2	32	77	5.31 Commun. 2010, 46, 4196 Chem.
34	2500	1.012	7.2	97	77	6.88 Commun. 2010, 46, 4196 Chem.—Eur. J. 2010,
35	2300	1.08	7.1	1	77	2.1 16, 14043
36	2300	1.08	7.1	60	776	5.53,7.8 Chem.—Eur. J. 2010, 16, 14043
37	2300	1.08	7.1	61	298980	0.399,0. Chem.—Eur. J. 2010, 16, 14043
38	2357	1.113	6.9	0.95	77	Cryst. Growth Des. 1.64 2010, 10, 3405
39	2357	1.113	6.9	17,31	77	Cryst. Growth Des. 3.98 2010, 10, 3405
40	2357	1.113	6.9	31	77	Cryst. Growth Des. 4.6 2010, 10, 3406
41	3000	1.36	6.36	1	77	Angew. Chem., Int. 2.25 Ed. 2010, 49, 5357
42	3000	1.36	6.36	33	77	Angew. Chem., Int. 6.24 Ed. 2010, 49, 5357
43	3000	1.36	6.36	90	298	Angew. Chem., Int. 0.667 Ed. 2010, 49, 5357
44	4118	2.35	7.3	1	77	1.4 Chem. Commun. 2011, 47, 9995
45	4118	2.35	7.3	44,60	77	5.6 Chem. Commun. 2011, 47, 9995
46	4118	2.35	7.3	60	77	9.2 Chem. Commun. 2011, 47, 9996
47	3989	2.173	8.14	1	77	Inorg. Chem. 2011, 50, 1.7 10528–10530
48	3989	2.173	8.14	60	77	Inorg. Chem. 2011, 50, 5.22 10528–10530
49	3394	1.38	5.8	1	78	2.42 Chem.—Eur. J. 2011, 17, 11162
50	3394	1.38	5.8	33,60	78	5.6 Chem.—Eur. J. 2011, 17, 11162
51	3394	1.38	5.8	60	78	7.5 Chem.—Eur. J. 2011, 17, 11163
52	4000	1.63	6.22	1	77	1.79 Angew. Chem., Int.

						Ed. 2010, 49, 5357 Angew. Chem., Int.
53	4000	1.63	6.22	45	77	6.65 Ed. 2010, 49, 5357 Angew. Chem., Int.
54	4000	1.63	6.22	90	298	0.785 Ed. 2010, 49, 5357 Angew. Chem., Int.
55	5109	2.13	6.09	1	77	1.87 Ed. 2010, 49, 5357 Angew. Chem., Int.
56	5109	2.13	6.09	50	77	7.32 Ed. 2010, 49, 5357 Angew. Chem., Int.
57	5109	2.13	6.09	90	298	1.01 Ed. 2010, 49, 5357
58	2970	1.25	5.9	1	78	2.39 Chem.—Eur. J. 2011, 17, 11162
59	2970	1.25	5.9	30,60	78	5.1 Chem.—Eur. J. 2011, 17, 11162
60	2970	1.25	5.9	60	78	6.7 Chem.—Eur. J. 2011, 17, 11163
61	6143	2.82	6.1	1	77	1.82 Nat. Chem. 2010, 2, 944
62	6143	2.82	6.1	56,70	77	9.95 Nat. Chem. 2010, 2, 944
63	6143	2.82	6.1	70	77	16.4 Nat. Chem. 2010, 2, 945
64	2620	1.07	4.15	1	77	2.5 Chem. Commun. 2011, 47, 4487
65	2620	1.07	4.15	20	77	6 Chem. Commun. 2011, 47, 4487
66	2100	0.795	10.1	1.2	77	2.2 J. Am. Chem. Soc. 2006, 128, 16876
67	2100	0.795	10.1	90	77	5.1,6.9 J. Am. Chem. Soc. 2006, 128, 16876
68	2100	0.795	10.1	90	298	0.94 J. Am. Chem. Soc. 2006, 128, 16876
69	2750	1.15	5	20	77	4 Chem. Eur. J. 2011, 17, 1837
70	2750	1.15	5	20	117	1.8 Chem. Eur. J. 2011, 17, 1837
71	1350	0.56	5.96	1	77	2.14 Chem. Commun. 2011, 47, 8304
72	1350	0.56	5.96	20	77	3.84 Chem. Commun. 2011, 47, 8305
73	1514	0.66	6.65	1	77	2.31 Chem. Commun. 2011, 47, 8306
74	1514	0.66	6.65	20	77	4.44 Chem. Commun. 2011, 47, 8307
75	922	0.38	7.1	1	77	1.98 Adv. Mater. 2005, 17, 2703
76	268	0.113	6.12	1	77	1.34 Chem. Commun. 2008, 44, 359
77	2590	1.05	7.74	1	77	1.68 Chem.—Eur. J. 2008, 14, 8812
78	2590	1.05	7.74	70	77	4.87,10 Chem.—Eur. J. 2008, 14, 8813
79	1630	0.64	4.5	1	77	1.27 Proc. Natl. Acad. Sci. U.S.A. 2006, 103, 10186
80	1630	0.64	4.5	55	77	3.01 Proc. Natl. Acad. Sci. U.S.A. 2006, 103, 10187
81	1630	0.64	4.5	1	77	1.3 J. Phys. Chem. C 2007, 111, 16131
82	1630	0.64	4.5	30	77	3.3 J. Phys. Chem. C 2007, 111, 16132
83	1630	0.64	4.5	60	298	0.13 J. Phys. Chem. C 2007, 111, 16133
84	512	0.203	6.2	1	77	1.04 Inorg. Chem. 2011, 50, 403
85	802	0.3	5.6	1	77	0.92 J. Am. Chem. Soc. 2007, 129, 9604
86	792	0.33	7.1	1	77	1.74 Adv. Mater. 2005, 17, 2703
87	792	0.33	7.6	1	77	2 Adv. Mater. 2005, 17, 2704
88	3670	1.52	7.05	1	77	1.79 Chem.—Eur. J. 2011, 17, 7251
89	3670	1.52	7.05	90	77	8.1,11.0 Chem.—Eur. J. 2011, 17, 7252
90	3670	1.52	7.05	90	298	0.5,1.19 Chem.—Eur. J. 2011, 17, 7253
91	922	0.38	6.9	1	77	1.94 Inorg. Chem. 2005, 44, 810

92	268	0.113	6.1	1	77	1.34 J. Phys. Chem. C 2008, 112, 17443
93	268	0.113	6.1	20	77	1.91 J. Phys. Chem. C 2008, 112, 17443
94	1407	0.67	6.8	1	77	2.34 J. Am. Chem. Soc. 2007, 129, 12368
95	1407	0.67	6.8	3.5	30	6.84 J. Am. Chem. Soc. 2007, 129, 12369
96	1407	0.67	6.8	45	300	0.25 J. Am. Chem. Soc. 2007, 129, 12370
97	1931	0.91	7	1	77	2.55 J. Am. Chem. Soc. 2007, 129, 12371
98	1931	0.91	7	3.5	30	7.89 J. Am. Chem. Soc. 2007, 129, 12372
99	1931	0.91	7	45	77	5.23 J. Am. Chem. Soc. 2007, 129, 12373
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101	2300	1	7.3	45	77	5.7 Angew. Chem., Int. Ed. 2008, 47, 4145
102	1239	0.62	6.1	1	77	2.18 Eur. J. Inorg. Chem. 2010, 3701
103	1154	0.62	4.5	50	77	3.6 J. Am. Chem. Soc. 2008, 130, 6119
104	1154	0.62	4.5	65	298	0.35 J. Am. Chem. Soc. 2008, 130, 6120
105	1154	0.62	4.5	60	200	1 J. Am. Chem. Soc. 2008, 130, 6121
106	1507	0.75	6.8	1	77	2.48 J. Am. Chem. Soc. 2011, 133, 17532–17535
107	1507	0.46~7		1	77	1.44 Inorg. Chem. 2011, 50, 1743
108	1507	0.75	6.8	1	77	2.27 Inorg. Chem. 2011, 50, 1744
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112	1630	0.64	4.5	1	77	1.3 J. Am. Chem. Soc. 2007, 129, 14176
113	1630	0.64	4.5	30	77	3.3 J. Am. Chem. Soc. 2007, 129, 14177
114	1630	0.64	4.5	60	298	0.13 J. Am. Chem. Soc. 2007, 129, 14178
115	783	0.39	8.3	1	77	1.75 J. Am. Chem. Soc. 2011, 133, 17532–17535
116	950	0.39	8.3	26.1	77	2.21 J. Am. Chem. Soc. 2006, 128, 726
117	870	0.39	8.8	30	77	2.8 Inorg. Chem. 2009, 48, 3882.
118	792	0.33	7.1	1	77	1.74 Inorg. Chem. 2005, 44, 810.
119	2885	1.18	4.8	1	77	1.15 Nature 2004, 427, 523.
120	2100	0.795	10.1	1	77	2.1 J. Am. Chem. Soc., 2006, 128, 16876.
121	2100	0.795	10.1	90	77	6.9 J. Am. Chem. Soc., 2006, 128, 16877.
122	2100	0.795	10.1	90	298	1.4 J. Am. Chem. Soc., 2006, 128, 16878.
123	792	0.33	7.1	1	77	1.74 Adv. Mater., 2005, 17, 2703; Chem.–Eur. J., 2005
124	922	0.38	6.8	1	77	1.98 Adv. Mater., 2005, 17, 2703; Chem.–Eur. J., 2005
125	1239	0.62	6.1	1	77	2.18 Adv. Eng. Mater. 2006, 8, 293
126	1507	0.75	6.8	1	77	2.48 J. Am. Chem. Soc. 2006, 128, 1304
127	802	0.3	4.31	1	77	0.93 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
128	676	0.34	5.96	1	77	1.23 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
129	837	0.33	4.99	1	77	1.45 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
130	988	0.39	4.51	1	77	1.54 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
131	813	0.32	4.46	1	77	1.42 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
132	382	0.15	4.45	1	77	0.75 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
133	400	0.16	7.5	1	77	1.12 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,

134	526	0.19	7.2	1	77	1.46 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
135	558	0.21	6.35	1	77	1.6 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
136	509	0.2	6.65	1	77	1.51 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,
137	163	0.07	7	1	77	0.54 Inorg. Chem. 2008, 47, 7936, Langmuir 2009, 25,