Computational Discovery for Crafting Multi-dimensional and Multi-functional Metal-Organic Framework Composites

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ABSTRACT

Rational design of multiple material components to create composite materials for synergistic enhancement is a crucial strategy in materials science. The combination of two-dimensional (2D) and three-dimensional (3D) metal-organic frameworks (MOFs) has great potential for creating multi-dimensional and multi-functional composites, expanding the material space for various applications. In this study, we developed a novel screening algorithm to construct 2D-MOF@3D-MOF composite structures using the intrinsic geometrical information of each MOF. Our algorithm was designed to prioritize synthesizability and identified several pairs of 2D-MOFs and 3D-MOFs. The screening results revealed that Ni-HHTP@UiO-66, a previously synthesized composite material, was among the potential candidates. Furthermore, the 2D-MOF@3D-MOF composite candidate that passed our algorithm exhibited superior mechanical strength compared to the mismatched composite. Our research advances the field of MOF by providing a practical screening algorithm for identifying suitable 2D-MOF@3D-MOF composite candidates and paves the way for the discovery of new materials with enhanced properties.
1. Introduction

Composite materials, consisting of two or more distinct materials with unique properties, have gained widespread attention for their ability to create new materials with enhanced functionalities.\textsuperscript{1, 2} The amalgamation of materials with different functionalities not only enhances individual properties but also creates novel properties with synergistic effects.\textsuperscript{3-6} Among the various materials, metal-organic frameworks (MOFs) have emerged as versatile and highly porous candidates for synthesizing composites due to their structural versatility, tunability, and crystalline ordered pores.\textsuperscript{7-9} Their facile synthesis process and a vast number of synthesized MOFs make them an ideal material to explore new composite materials.\textsuperscript{10-14} To date, researchers have combined MOFs with a wide range of compounds, including metal nanoparticles,\textsuperscript{15-20} metal oxides,\textsuperscript{21-24} quantum dots,\textsuperscript{25-28} carbon nanotubes,\textsuperscript{29-32} and polymers.\textsuperscript{33, 34} For instance, the incorporation of MOFs into polymer matrix results in composites with improved chemical and mechanical stability when compared to pure MOFs.\textsuperscript{33} The composites of MOFs with metal nanoparticles or metal oxides lead to not only enhanced stability but also boosted catalytic activity, resulting in a synergistic effect.\textsuperscript{35}

The synthesis and characterization of MOF and MOF composites (here, MOF@MOF) have been extensively studied, and their potential applications have been thoroughly evaluated.\textsuperscript{36-41} However, for practical applications, a design-oriented approach is essential to optimize the performance of composite materials by considering the combination of materials that have the potential to improve performance and maximize synergistic effects. For example, a special core/shell composite was created using a large pore MOF (UiO-66-NH\textsubscript{2}) as the core surrounded by a small pore MOF (ZIF-8) as the shell.\textsuperscript{42} The hybrid UiO@ZIF membrane showed improved hydrophobicity, excellent CO\textsubscript{2} permeability (710\% higher than single membrane), and
substantial CO$_2$/N$_2$ selectivity (50% higher than single membrane). Another example is the synthesis of Matryoshka-type of MOF composite, consisting of multiple layers of ZIFs, with ZIF-8 serving as the shell MOF and ZIF-67 as the core MOF. The hydrogen spillover phenomenon was boosted using the composite materials via ZIF-8 shell functioned as a spatial ruler, determining the farthest possible travel distance of dissociated hydrogen atoms, while the ZIF-67 core acted as a detector of hydrogen atoms via hydrogenolysis.

By adopting a strategy to mix MOFs with vastly different properties, it is expected to enhance performance or create new synergistic effect by synthesizing a multi-functional MOF composite. From this perspective, incorporating materials with varied dimensional characteristics (i.e. multi-dimensional) is a noteworthy approach for anticipating novel synergistic effects. For example, Das et al. introduced a two-dimensional covalent-organic framework (2D-COF) named H$_2$P-DHPh onto 3D-MOF (UiO-66), resulting in an innovative composite material that demonstrated exceptional H$_2$/CO$_2$ selectivity. In the field of energy storage, it has become prevalent to utilize composite materials that combine disparate dimensional components, such as decorating 0D metal oxide nanoparticles with 2D conductive graphene or MXene. These materials have shown noteworthy enhancements as electrode materials with high capacity and excellent cycling stability. Therefore, synthesizing multi-functional and multi-dimensional MOF composite materials represents a promising approach for achieving synergistic enhancements.

MOFs can be also classified based on their dimensionality, which influences their intrinsic functionalities. For instance, 3D-MOFs generally possess large pore volumes and are commonly used for gas storage, water harvesting, and drug delivery. On the other hand, 2D-MOFs are constructed through van der Waals interactions and can serve as membranes for gas separation. Recently, conductive 2D-MOFs with transition metals and highly
conjugated organic linkers have been gaining attention due to their remarkable electrical conductivity. Therefore, 2D-MOFs have advantages in areas not only gas separation but also chemical sensing and super-capacitors. It is notable that we can expect a completely new synergistic effect or improved property by synthesizing a multi-dimensional and multi-functional 2D-MOF@3D-MOF composite which have different properties. Recently, our group and co-workers successfully synthesized a 2D-MOF@3D-MOF composite material utilizing Ni-HHTP (i.e. Ni$_3$(HHTP)$_2$·2[Ni$_3$(HHTP)]·nH$_2$O, HHTP = 2,3,6,7,10,11-hexahydroxytriphenylene) as a conductive 2D-MOF and UiO-66-NH$_2$ as porous 3D-MOF. Remarkably, this composite material exhibited an incredibly enhanced chemiresistive sensing response and recovery to toxic H$_2$S gas due to the synergistic effect at the interfaces. As such, novel 2D-MOF@3D-MOF composites possess the potential to exhibit synergistic property and exploring various combinations of 2D-MOF@3D-MOF composite is crucial as it has the possibility to open up new areas of research.

To expediently search for 2D-MOF@3D MOF pairs, computational screening can facilitate identifying ideal candidate pairs for the MOF composites. Our group has previously developed a computational screening algorithm that can predict 3D-MOF@3D-MOF and 3D-MOF@3D-COF composites. Despite these achievements, there is currently no existing algorithm to predict clean 2D-MOF@3D-MOF candidates using atomic-scale bottom-up insights. In this work, we have developed a computational screening algorithm that exploits the chemical bonding between the organic linker of one MOF and the metal node of the second MOF to create 2D-MOF@3D-MOF composites with superior structural stability. Thus, our advanced screening algorithm enables the creation of highly stable and user-desired 2D-MOF@3D-MOF composites.
In this study, we developed a novel computational screening algorithm that utilizes geometrical information of each MOF in the atomic-level to predict potentially synthesizable 2D-MOF@3D-MOF pairs. Specifically, we selected two 2D-MOFs, Ni-HHTP and CuBDC (copper 1,4-benzenedicarboxylate), as the fixed candidates for one MOF, and screened a vast database of about 90,000 3D-MOFs to identify the ideal candidates. Through the application of our developed screening algorithm, we successfully identified highly synthesizable 2D-MOF@3D-MOF candidates. The identified 2D-MOF@3D-MOF composite candidate demonstrated superior mechanical strength compared to the mismatched composite candidate, and our results demonstrate a new approach for the rational design of multi-dimensional and multi-functional composite materials.

2. Computational Screening Methods

2.1 Database Preparation

The 2D-MOF and 3D-MOF database used in this study were prepared as shown in Figure 1. For the choice in the 2D MOFs, CuBDC was selected as a candidate due to its outstanding gas separation performance. (Figure 1a-b) Several research work has shown that CuBDC 2D sheets with lateral dimensions in the nanometer thickness exhibited exceptional CO$_2$ separation performance from CO$_2$/CH$_4$ gas mixtures and a desirable increase in separation selectivity with pressure when incorporated into polymer composites or dispersed within a continuous polymer matrix (i.e. mixed matrix membranes).$^{79-81}$ The CuBDC structure was taken from Carson et al. (refcode: PUYREH)$^{82}$ and the reported unit cell parameter was (11.4143 Å × 14.2687 Å × 7.78 Å) with angle of $\alpha = \gamma = 90^\circ$ but $\beta = 108.1^\circ$. (Figure 1a) After removing unbound solvent, single layer was extracted by cleaving surface through ($\overline{2}01$). (Figure 1b)
The second 2D-MOF, Ni-HHTP, was chosen for its remarkable electrical conductivity, which makes it a promising candidate for various electrical applications. (Figure 1c-d) The conductive Ni-HHTP has been constructed by combining transition metal, nickel, and conjugated organic linker, HHTP. The strong charge delocalization through both extended \( \pi \)-\( d \) conjugation and \( \pi \)-\( \pi \) orbital overlap facilitated outstanding electrical property in the Ni-HHTP.\(^{64-67}\) The Ni-HHTP structure was prepared by referring to Hmadeh et al. (refcode: SETGUV)\(^{83}\) As shown in Figure 1c, the Ni-HHTP possessed honeycomb topology and lattice parameter of (22.13 Å × 22.13 Å × 13.31 Å) with \( \alpha = \beta = 90^\circ \) but \( \gamma = 120^\circ \). The original structure file contained unnecessary structures such as discrete complex and solvents attached to the axial position of the Ni metal. We hypothesized that the 2D-MOF is in a fully activated state, thereby the extraneous structures were manually removed. The extracted single layer was slightly bent because of external solvents, so the geometrical optimization was conducted using density functional theory (DFT) calculation. The single layer was put alone on the cell box with large vacuum. (22.13 Å × 22.13 Å × 25 Å) The DFT optimization resulted in a structurally feasible flattened single layer of Ni-HHTP, which was utilized for subsequent screening process. (Figure 1d, see computational details in Supporting Note 1)

In the case of 3D-MOFs, 91,805 MOF structure data were prepared from the Cambridge Structural Database (CSD)\(^{10}\) via ConQuest software (Figure 1e). After a removal of floating solvents (e.g. charge balancing solvents), the MOFs that are not fully connected (i.e. 0D, 1D, 2D) were identified and removed from the database using our in-house code. After that, the number of structures was reduced to the 31,227. The cleaved structures of 3D-MOFs were utilized through the screening process because core-shell composite materials have been synthesized through tight interfacial bonding in their adhered interface. Here, four surfaces, (100), (010),
The organic ligands containing carboxylic acid are representative compounds most commonly used in MOF synthesis. In this research, only MOFs containing carboxylic acid were considered and extracted. Finally, 8,949 cleaved 3D-MOF structures were used as a final 3D-MOF database for the screening.

(Figure 1e)

2.2 Identification of Connection points

Lattice matching and chemical connection point matching have been considered as crucial algorithms in the previous 3D-MOF@3D-MOF and 3D-MOF@3D-COF screening studies. In these studies, it is notable to mention that lattice parameter matching algorithm was important because they considered 3D structures. However, we exclusively employed monolayer 2D-MOF that does not exhibit any stacking configuration in the planar direction. This implies that a 3D lattice cannot be defined to the single-layered 2D-MOF, thereby rendering lattice parameter matching algorithms inapplicable. The decrease in dimensionality leads to a reduced number of variables to be considered, which consequently results in the predominant utilization of connection point matching algorithm for the 2D-MOF@3D-MOF system. This unique aspect of 2D-MOF@3D-MOF systems may allow for a more flexible approach to materials screening, making our algorithm a powerful tool for finding suitable composite candidates. We hypothesized that the core-shell composite material can be formed when the metal cluster of a 3D-MOF and organic ligand of a 2D-MOF are bonded in their interface. In other words, the carboxylic acid associated with metal cluster of the 3D-MOF should be replaced by the organic ligand of the 2D-MOF. As a result, the carboxylic acid connected with metal cluster of the 3D-
MOF and the organic ligands in 2D-MOF were defined as the connection point in the 3D-MOF and 2D-MOF, respectively. (Figure 2)

As illustrated in Figure 2a, for the CuBDC 2D-MOF, the carboxylic acid in the BDC linker served as the connection point. And for the Ni-HHTP 2D-MOF, the hydroxy group in the HHTP linker was considered as the connection point (Figure 2d). It has been established in prior research that the hydroxy group in HHTP linker has the capability to form a strong bonding with Zr metal cluster of UiO-66-NH2.76 The connection points with the 3D-MOF were identified and characterized based on their z-coordinate on the same cleaved surface. The demonstration of the connection point identification process was shown in Figure 2b and Figure 2e using examples of IRMOF-8 (refcode: EDUTUS) and UiO-66 (refcode: RUBTAK), respectively. Four and twelve connection points were obtained from the (100) cleaved surface of IRMOF-8 and (111) surface of UiO-66, respectively. Then, the geometrical information of connection points of 2D-MOF and 3D-MOF were calculated to see whether they could match or not. (Figure 2c and 2f) The details of connection point matching process will be discussed in subsequent section.

2.3 Connection points matching algorithm

It was postulated that the chemical connection point matching would occur if two geometrical parameters of the connection points were compatible: (1) the distance between two connection points of 2D-MOF ($d_{2D}$) and 3D-MOF ($d_{3D}$), and (2) the angle defined by the vector between two connection points of 3D-MOF ($\overrightarrow{d_{3D}}$) and the vector between two oxygen atoms in a single connection point of 3D-MOF ($\overrightarrow{d_{3D,0}}$). The schematic illustration of connection point matching algorithm is shown in Figure 3. The distance between two neighboring connection points in 2D-MOF and 3D-MOF were indicated as $d_{2D}$ and $d_{3D}$, respectively. The value of $d_{2D}$
in CuBDC and Ni-HHTP was equal to 10.788 Å (Figure 3a) and 22.13 Å (Figure 3b), respectively. The value of $d_{3D}$ can vary depending on the two choices in the connection points within the plane of the 3D-MOF. (Figure S1) Distance matching was conducted that the difference between $d_{2D}$ and $d_{3D}$ must be smaller than distance threshold (i.e. $\varepsilon$). Meanwhile, despite any disparities in the number of connection points between 2D-MOF and 3D-MOF, a core-shell structure is feasible to be synthesized.\textsuperscript{77, 85, 86} Thus, the distance of integer and half-integer multiples (here, we defined as $\delta$) of the $d_{2D}$ were considered as potential candidates. To sum up, the distance matching algorithm can be represented as an equation, $\left| \frac{d_{2D} - d_{3D} \times \theta}{d_{2D}} \right| < \varepsilon$.

The distance threshold, $\varepsilon$, was fixed as ±4 % of $d_{2D}$ and the multiples, $\delta$, was varied as 0.5, 1.0, 1.5, 2.0 and 2.5.

Furthermore, angle information of 3D-MOF was employed in connection point matching. A vector between two oxygen atoms in a single connection point of 3D-MOF (i.e. single carboxylic acid) was defined as a $\overrightarrow{d_{3D,O}}$. (Figure 3) The angle between $\overrightarrow{d_{3D,O}}$ and $\overrightarrow{d_{3D}}$ vectors must be perpendicular to be matched with CuBDC (i.e. $\overrightarrow{d_{3D,O}} \perp \overrightarrow{d_{3D}}$, Figure 3a), but parallel for the Ni-HHTP (i.e. $\overrightarrow{d_{3D}} \parallel \overrightarrow{d_{3D,O}}$, Figure 3b). In other words, the angle should be 90° and 0° (or 180°) for CuBDC and Ni-HHTP, respectively. To allow small deviation of the bonding geometry, strict angle threshold was set as ±1°. The 3D-MOFs which passed the both criteria for distance and angle matching were regarded as the candidate MOFs which can form 2D-MOF@3D-MOF composite with CuBDC or Ni-HHTP.

3. Results and Discussion

3.1 Computational screening results
According to our screening algorithm, we identified 11 and 102 3D-MOFs that are promising synthesizable candidates for CuBDC@3D-MOF and Ni-HHTP@3D-MOF, respectively. The full refcode name and the cleaved surface of the candidates according to the $\delta$ values are tabulated in Table S1.

The representative illustration examples are displayed in Figure 4. As shown in Figure 4a, the CuBDC@EDUTUS core-shell composite was predicted to be an appropriate candidate. The MOF with refcode EDUTUS is IRMOF-8 which is known as isoreticular series of IRMOF-1. EDUTUS is constructed from octahedral Zn-O-C clusters and naphthalene-2,6-dicarboxylate (2,6-NDC) and has a primitive cubic structure. Upon analyzing the EDUTUS along (100) surface, a pair of carboxylic acids were found to serve as the connection point with a distance value of 21.278 Å combined with $\delta = 0.5$. (i.e. 10.639 Å) This distance is slightly shorter than the distance of CuBDC (10.788 Å), with a mismatch ratio of 1.38%. Following the distance matching, an angle matching was conducted, and (100) surface of EDUTUS was considered as a suitable surface. Several 3D-MOFs were also identified as potential candidates for CuBDC. These candidates have the same metal cluster and topology as EDUTUS but use different types of organic linkers. Spanopoulos et al. modified the NDC linker in IRMOF-8 by functionalizing two hydroxyl groups, resulting in OH-IRMOF-8 (SERBUO). The distance mismatch between SERBUO and CuBDC was calculated to be only 1.11%. Furthermore, Prasad et al. and Barman et al. synthesized IRMOF-8 analogous structures using 4-(2-carboxyvinyl)-benzoic acid (CVB) and 2,6-azulenedicarboxylate (2,6-azd) organic linkers, respectively. (refcodes are GEBPEK and BOQQAB, respectively) GEBPEK and BOQQAB have distance mismatch errors of 0.92 % and 0.14 %, respectively, indicating that these 3D-MOFs should also be matched with CuBDC.
Meanwhile, a larger number of candidates were found in the Ni-HHTP screening compared to the CuBDC. RUBTAK, which is one of the most famous MOF (UiO-66), was extracted as proper candidate of Ni-HHTP. The RUBTAK is composed by 12-coordinated Zr-oxo metal cluster and BDC organic linkers and has attention for its high surface area as well as high thermal stability.91, 92 By cleaving RUBTAK along (111) surface, two carboxylic acids were identified as connection points with the distance, 14.637 Å. One and a half times of the distance value (21.956 Å) was matched with distance of Ni-HHTP (22.13 Å) with only 0.79% of error. After passing through the distance matching criteria, angle matching was conducted. As a result, angle difference was calculated as 0° and RUBTAK was considered as promising candidates along the (111) surface. The core-shell structure of Ni-HHTP@RUBTAK was shown in Figure 4b. Interestingly, RUKDIM, which consists of the Zr metal cluster same as RUBTAK, was also derived as an appropriate candidate. RUKDIM is isostructural series of RUBTAK, but have an elongated organic linker, named 4,4′-ethynylenedibenzoate, when compared to that of BDC.93 RUKDIM was cleaved through (111) surface and the distance value (21.382 Å) was matched to the Ni-HHTP within 3.38% error. Ni-HHTP@RUKDIM core-shell can be crystalized with 1:1 ratio of connection points.

It is worth mentioning that the Ni-HHTP@RUBTAK composite pair was successfully synthesized in previous experimental study.76 The tight interfacial bonding of the HHTP ligand to the Zr metal cluster at the interface was confirmed through comprehensive characterization techniques such as transmission electron microscopy (TEM), cryogenic electron microscopy (Cryo-EM), and electron paramagnetic resonance (EPR). Therefore, the use of the screening algorithm is expected to provide practical assistance in the synthesis of 2D-MOF@3D-MOF
composites. Consequently, the proposed 2D-MOF@3D-MOF candidate pairs in this study are believed to possess the potential for synthesis.

3.2 Mechanical strength of well-matched 2D-MOF@3D-MOF structures

Our research endeavors to introduce an advanced algorithm capable of generating a highly compatible 2D-MOF@3D-MOF composite candidate featuring a tight chemically bonded molecular structure. To appraise the structural integrity of the composite materials, two specific composite materials, namely Ni-HHTP@RUBTAK and Ni-HHTP@WIZMAV, have been selected as well-matched and mis-matched candidates, respectively (Figure 5a and 5c). Although WIZMAV shares a similar iso-reticular structure with RUBTAK, namely UiO-67, it is deemed a mis-matched candidate due to the elongated length of its 4,4'-biphenyldicarboxylate linker, leading to a distance error of 14.06%. (with a distance value of 19.018 Å)

First, net bonding energy in the interface were calculated. Previous study has indicated that the bonding energy between a HHTP linker and a Zr metal cluster is –536.59 kJ/mol. The net bonding energy per unit cell area of Ni-HHTP@RUBTAK and Ni-HHTP@WIZMAV were calculated as –0.122 and –0.027 kJ/mol Å⁻², respectively (Table 1, Figure S2). We reveal that Ni-HHTP@RUBTAK is expected to exhibit significantly enhanced structural stability compared to Ni-HHTP@WIZMAV, as evidenced by its net bonding energy being 4.52 times stronger, resulting in a more stable composite. Additionally, we also quantitatively analyzed the mechanical strength of each composite by applying strain and observing the corresponding stress changes using molecular dynamics (MD) simulation (Figure 5, see computational details in Supporting Note 1). The Young’s modulus for Ni-HHTP@RUBTAK and Ni-HHTP@WIZMAV were calculated as 90.8 and 52.8 GPa, respectively. It is noteworthy that Ni-HHTP@RUBTAK
exhibits higher mechanical strength compared to Ni-HHTP@WIZMAV, as it is less prone to deformation. Our proposed algorithm, therefore, provides a comprehensive solution to the synthesis of 2D-MOF@3D-MOF composite candidates with high structural stability and strong mechanical strength at the interface, evaluated through the net bonding energy per unit cell area and Young's modulus.

4. Conclusion

In this research, we have developed a novel and practical screening algorithm for 2D-MOF@3D-MOF candidates using intrinsic geometrical information of connection points. The algorithm was designed with strict criteria to ensure high synthesizability, which includes a distance error of no more than 4% and an angle error of only up to 1°. Computational screening was performed, and the results showed 11 and 102 3D-MOFs for CuBDC@3D-MOF and Ni-HHTP@3D-MOF, respectively. Representative candidates, CuBDC@EDUTUS (IRMOF-8) and Ni-HHTP@RUBTAK (UiO-66), were modeled as core-shell structures, and high structural compatibility was observed through net bonding energy and mechanical strength calculation. In particular, the reliability of our screening algorithm was validated by the fact that RUBTAK, which was synthesized as composite material with Ni-HHTP in previous study, was predicted by our screening. The 2D-MOF@3D-MOF composite can offer the ability to control the crystal growth of the 2D-MOF and to adjust geometrical properties such as the stacking arrangement and interlayer distance of the 2D sheets. Furthermore, creating new chemical bonds at the 2D-MOF@3D-MOF interface may enhance intrinsic characteristics such as the electronic structure or thermal stability. Our study aims to inspire the synthesis of multi-dimensional and multi-functional 2D-MOF@3D-MOF composites and contribute to the discovery of new materials.
Figure 1. Database Construction. (a) Bulk structure of CuBDC obtained from Carson et al. (refcode: PUYREH)\textsuperscript{82}. (b) Single layer structure of CuBDC. (c) Bulk structure of Ni-HHTP obtained from Hmadeh et al. (refcode: SETGUV)\textsuperscript{83}. (d) Single layer structure of Ni-HHTP. (e) Process involved in preparing the 3D-MOF database. Atom color is matched as follows: light blue: Ni, red: O, grey: C, white: H, blue: N, coral: Cu.
Figure 2. Identification of connection points in 2D-MOFs and 3D-MOFs. (a) Identified connection points in CuBDC single layer. (b) Identified connection points in IRMOF-8 through (100) surface. (c) Illustration of well-matched connection points between CuBDC and IRMOF-8 ($\delta = 0.5$) (d) Identified connection points in Ni-HHTP single layer. (e) Identified connection points in UiO-66 through (111) surface. (f) Illustration of well-matched connection points between Ni-HHTP and UiO-66 ($\delta = 1.5$) The blue and purple spheres indicate the connection points in 2D-MOF and 3D-MOF, respectively.
Figure 3. Connection point matching algorithm. Well-matched examples of (a) CuBDC and (b) Ni-HHTP, respectively. The large blue and purple spheres indicate the connection points in 2D-MOF and 3D-MOF, respectively. $\overline{d_{2D}}, \overline{d_{3D}}$ and $\overline{d_{3D,0}}$ are the vector between two connection points of 2D-MOF, the vector between two connection points of 3D-MOF and the vector between two oxygen atoms in a single connection point of 3D-MOF, respectively. $\delta$ indicates multiplier and $\varepsilon$ represent distance threshold, respectively. The illustrations presented in this figure are examples when the value $\delta$ is equal to 1.0.
Figure 4. Ideal computational 2D-MOF@3D-MOF structures. (a) CuBDC@EDUTUS and (b) Ni-HHTP@RUBTAK. The blue spheres indicate the well-matched connection points in their interface. Each color is matched as follows: light blue: Ni, red: O, grey: C, white: H, coral: Cu, sky blue: Zr.
Table 1. Net bonding energy per unit cell area for the Ni-HHTP@RUBTAK and Ni-HHTP@WIZMAV

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Figure 5. Mechanical strength calculation. (a) The initial structure of (a) Ni-HHTP@RUBTAK and (c) Ni-HHTP@WIZMAV. The final structure after applying strain through molecular dynamics (MD) simulation of (b) Ni-HHTP@RUBTAK and (d) Ni-HHTP@WIZMAV. Blue and purple represent 2D-MOF and 3D-MOF, respectively. (e) Stress-strain curve for the Ni-HHTP@RUBTAK and Ni-HHTP@WIZMAV. Trendline is plotted as dotted line and the slope indicate young’s modulus.
ASSOCIATED CONTENT

Supporting Information

The supporting Information is available free of charge at

Description of settings for DFT and MD simulation, connection points, whole refcode names of screening results, structural illustration of mechanical strength simulation, Table S1, Figure S1-S2, and related references (PDF)

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Notes

The authors declare no competing financial interest.

AUTHOR CONTRIBUTIONS

M. J. and J. K. conceived the project. M. J. performed the calculations and conducted the analysis and wrote the paper. J. K. supervised the project. All authors read and approved the manuscript.

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