

# A Short Note on the Properties of Metal-Doped Covalent Organic Frameworks

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## DESCRIPTION

Covalent organic frameworks are distinctive for their extremely open design and attractive to be used as promising gas adsorption and storage carriers. During this work, density functional theory calculations are performed to analyze the properties of metal-doped covalent organic frameworks and their interactions with the SO<sub>2</sub> gas molecule. It's found that one metal atom doped at the highest of phenyls within the Tetra(4-dihydroxyborylphenyl) Silane (TBPS) building block of covalent organic frameworks will simply lose its valence electrons and might be positively charged. The SO<sub>2</sub> gas molecule can be stably absorbed onto the metal-doped covalent organic frameworks. The absorbed SO<sub>2</sub> molecule interacts with Li, Na, K, and Sc metal-doped covalent organic frameworks by the dominant donor-acceptor delocalization between the lone pair of an oxygen atom inside Sulfur dioxide and 1-center non-Lewis lone pairs of the doped metal atom.

Sulfur dioxide gases, primarily resourced from industrial activities, are referred to as the main source of air pollution leading above all to acid smog formation and air rain. Reducing sulfur dioxide emissions has become one of the foremost necessary social and environmental challenges. It should be detected that adsorption by porous nanomaterials is recognized as an efficient and economical approach for the capture of low concentration SO<sub>2</sub> from mixture gases [1]. Covalent Organic Frameworks (COFs) are ideal porous materials for gas capture because of their low density, stability, and huge surface area. Target valence organic framework porous materials are designed and synthesized for sulfur dioxide gas adsorption and separation.

Doping of metals into covalent organic frameworks is one of the foremost effective modifications of covalent organic frameworks for gas capture. Experimental and theoretical studies are distributed to explore the doping of metals into the organic frameworks so as to boost their capture of hydrogen and carbon dioxide gases. Medina et al. doped metal palladium clusters onto COF-1 materials and increased their hydrogen storage properties [2]. Palo-Nieto et al. reported the doping of platinum clusters onto valence organic frameworks and investigated the hydrogen result reaction mechanisms [3]. Kaneko et al. reported carbon dioxide natural process properties in 2 isostructural azine-linked covalent organic frameworks supported 1,3,5-triformyl aromatic

hydrocarbon (AB-COF) and 1,3,5-triformylphloroglucinol (ATFG-COF) and hydrazine building units [4]. However, there are few studies focused on SO<sub>2</sub> gas adsorption and separation on the metal-doped covalent organic frameworks and the interactions between the metal-doped organic frameworks and SO<sub>2</sub> gases. In this work, density functional theory calculations are performed to analyze the properties of metal-doped covalent organic frameworks and their interactions with SO<sub>2</sub> gas. Considering the doping result of alkali metals and transition metals into the organic framework for hydrogen and carbon dioxide, we tend to choose alkali (Li, Na, and K) and transition metals (Sc) doped into covalent organic frameworks and investigated the properties of the metal-doped covalent organic frameworks and their interactions with the SO<sub>2</sub> gas molecule.

The cluster model of covalent organic frameworks consisting of the tetra(4-dihydroxyborylphenyl) silane (TBPS) and 2,3,6,7,10,11-hexahydroxy triphenylene (HHTP) building blocks elite from COF-105 is adopted to represent the important structure of COF-105 [5]. The functional groups of the covalent organic framework cluster model are saturated by hydrogen. Considering the various doping sites, alkali (Li, Na, and K) and transition (Sc) metals were doped into the cluster model of COF-105.

## REFERENCES

- Balmond EI, Coe DM, Galan MC, McGarrigle EM. Mechanisms of enzymatic CO bond cleavages in deoxyhexose biosynthesis. *Angew Chem Int Ed.* 2012;51: 9152.
- Medina S, Harper MJ, Balmond EI, Miranda S. Stereoselective Glycosylation of 2-Nitrogalactals Catalyzed by a Bifunctional Organocatalyst. *Org Lett.* 2016;18: 4222.
- Palo-Nieto C, Sau A, Williams R, Galan MC. Cooperative Brønsted Acid-Type Organocatalysis for the Stereoselective Synthesis of Deoxyglycosides. *J Org Chem.* 2017;82: 407.
- Kaneko M, Herzon SB. Scope and Limitations of 2-Deoxy- and 2,6-Dideoxyglycosyl Bromides as Donors for the Synthesis of  $\beta$ -2-Deoxy- and  $\beta$ -2,6-Dideoxyglycosides. *Org Lett.* 2014;16: 2776.
- Issa JP, Bennett CS. A Reagent-Controlled SN<sub>2</sub>-Glycosylation for the Direct Synthesis of  $\beta$ -Linked 2-Deoxy-Sugars. *J Am Chem Soc.* 2014;136: 5740.

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