

# F-gas adsorption in pillared graphene materials. Insights from molecular simulations.

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## Abstract

Fluorinated gases (F-gases) such as SF<sub>6</sub>, CF<sub>4</sub> and their gas mixtures with N<sub>2</sub> are well known insulators used in many industrial applications. The consideration of this fluid mixture is highly relevant for the reduction of greenhouse gases emission and in the field of electrical power transmission equipment. For example, SF<sub>6</sub> has to be recovered due to its high global warming potential (SF<sub>6</sub> shows one of the highest global warming potentials, 24000 times higher than CO<sub>2</sub>, and has a very long atmospheric lifetime) and for saving costs. Adsorption-based processes using porous carbon materials are considered as an efficient way to achieve SF<sub>6</sub> recovery [1]. We report a computational assessment of the adsorption uptake and separation performances of a set of three-dimensional porous carbon nanotube networks (PNN) and pillared graphene materials for SF<sub>6</sub>/N<sub>2</sub>, SF<sub>6</sub>/CF<sub>4</sub> and CF<sub>4</sub>/N<sub>2</sub> fluid mixtures, as well as the adsorption uptake for the pure fluids [2].

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## References

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- [2] Skarmoutsos, I.; Koukaras, E. N.; Galiotis, C.; Froudakis, G. E.; Klontzas, E. *Microporous Mesoporous Mater.*, 307 (2020), 110464.

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