

## The Role of h-BN on the Iodine Gas Sorption of Cu under High Humidity

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### 1. Introduction

The management of radioactive iodine gas I<sub>2</sub>(g) is critical for environmental safety in nuclear engineering, particularly during the handling of spent fuel and radioisotopes. Currently, activated carbon (AC) [1] or silver-exchanged zeolites (AgZ) [2] are primarily used to capture I<sub>2</sub>(g) during the chemical processing of iodine (I<sub>2</sub>)-containing nuclear materials.

Recently, copper (Cu) has been identified as a promising alternative to Ag-based sorbents for I<sub>2</sub>(g) capture due to its high affinity for I<sub>2</sub>, cost-effectiveness, and non-toxicity. However, the impact of humidity has not yet been systematically studied, in addition to the effect of temperature on I<sub>2</sub>(g) sorption.

In this study, we investigated the I<sub>2</sub>(g) sorption properties of Cu particles supported by hexagonal boron nitride (h-BN) under dry and humid conditions at various temperatures. The role of h-BN in enhancing the I<sub>2</sub>(g) sorption of Cu is discussed.

### 2. Experimental Procedures

Cu<sup>0</sup>@h-BN composites were synthesized via a solvothermal reduction method, wherein Copper (II) nitrate trihydrate, h-BN powder, and ethylene glycol were thoroughly mixed and transferred in a Teflon-lined stainless-steel reaction autoclave and heated at 200°C for 24h. The synthesized composite was then vacuum-dried at 60°C for 12h.

Non-radioactive solid I<sub>2</sub> crystals were used for the I<sub>2</sub>(g) sorption test in a sealed desiccator, heated in an oven at temperatures ranging from 75°C to 250°C. Humidity was controlled using saturated salt solutions of NaCl and KNO<sub>3</sub> to maintain constant relative humidities of 75% and 85%, respectively. After 24h of exposure, the mass gain was measured once the samples cooled, and the results were compared with blank control tests carried out without I<sub>2</sub> exposure.

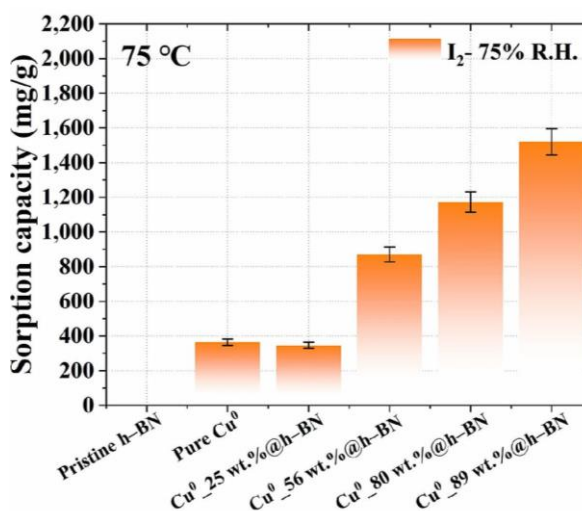
To characterize the Cu<sup>0</sup>\_x wt.%@h-BN composites, powder X-ray diffraction (PXRD), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) in backscattered-electron (BSE) mode equipped with energy-dispersive X-ray spectroscopy (EDS), the Brunauer-Emmett-Teller (BET) method, thermo-gravimetric analysis-mass

spectrometry (TG-MS), and X-ray photoelectron spectroscopy (XPS) were employed to assess their structural and thermal properties.

### 3. Results

Compared with pure Cu (Cu<sup>0</sup>), Cu<sup>0</sup>@h-BN composites exhibited reduced binding energies for the Cu 2p, B 1s, and N 1s peaks. These shifts indicate a redistribution of electron density through electron transfer at the interface of Cu and h-BN, creating additional active sites for interactions between Cu and I<sub>2</sub> molecules. The metal-support interaction (MSI) effect in Cu<sup>0</sup>@h-BN composites thus plays a crucial role in enhancing both the performance and stability of the material for I<sub>2</sub>(g) capture.

Experiments conducted at 75% and 85% relative humidity demonstrated that Cu<sup>0</sup>@h-BN composites maintained strong I<sub>2</sub>(g) sorption capabilities, whereas pure Cu<sup>0</sup> experienced a significant performance drop due to water-induced passivation. The presence of h-BN prevents excessive water sorption, thereby preserving the reactivity of Cu sites. The composite material reliably captures I<sub>2</sub> even at moderate temperatures below 100°C without rapid deactivation, underscoring the crucial role of h-BN in protecting Cu<sup>0</sup> against moisture. Furthermore, the h-BN substrate stabilizes Cu particles and promotes faster I<sub>2</sub>(g) capture.



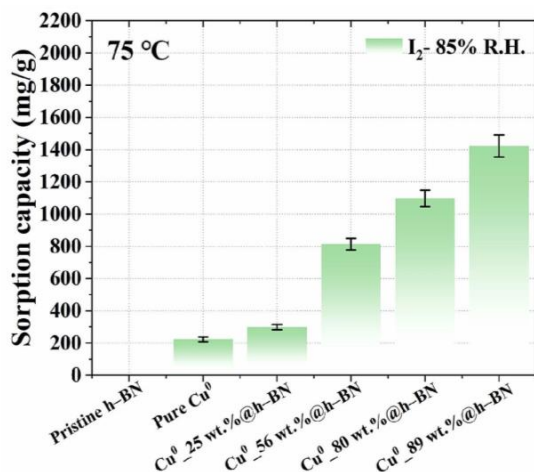


Fig. 1. The sorption performance of Cu<sup>0</sup>@h-BN composites under humid conditions at 75% R.H. and 85% R.H.

### 3. Conclusions

This study demonstrates that the interactions between Cu and h-BN modify the electronic and chemical properties of the composite material. In particular, under humid conditions at moderate temperatures below 100°C, Cu<sup>0</sup>@h-BN composites maintain stable I<sub>2</sub> sorption capabilities. The MSI effect within Cu<sup>0</sup>@h-BN composites is proposed as a vital mechanism for improving the performance and stability of these materials in I<sub>2</sub>(g) capture applications.

### REFERENCES

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