



Showcasing research from Dr. Buchsbaum and team at Lawrence Livermore National Laboratory, USA.

Mechanisms and effects of gas intercalation into ionic liquids confined within charged nanoscale volumes

Understanding gas behavior within confined ionic liquids (ILs) is critical for advancing energy, separation, and sensing technologies. Our work combines molecular dynamics simulations and experimental validation to explore the mechanisms governing the solubility and arrangement of  $\text{CO}_2$ ,  $\text{N}_2$ , and  $\text{O}_2$  in 1-butyl-3-methylimidazolium hexafluorophosphate confined within charged carbon nanotubes (CNTs). The findings reveal how confinement, CNT charge state, and IL properties influence gas selectivity and electrochemical signal changes, providing helpful insights to next-generation electrochemical systems designed for gas sensing and separation applications.

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See Fikret Aydin, Steven F. Buchsbaum, *et al*, *Nanoscale*, 2025, **17**, 7813.