

# Workshop on Xenon Detector $0\nu\beta\beta$ Searches: Steps Towards the Kilotonne Scale

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## Material structures and intermolecular forces relevant to adsorption-based xenon capture

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Given that xenon production by cryogenic distillation is prohibitory in cost and insufficient in quantity to provide for the next generation of xenon detectors, adsorption of xenon onto porous materials may be a viable alternative. Activated carbons and zeolites are possible adsorbent candidates. However, the non-specific intermolecular interactions between these materials and xenon afflict them with poor selectivity for xenon against other atmospheric gases. Intelligently designed materials containing pores tailored to the size of the xenon atom may prove to be superior adsorbents due to their high selectivity conferred by stronger attractive interactions with xenon compared to other gas species. Certain metal-organic frameworks (MOFs) with appropriately sized pores have shown promise for highly selective capture of large volumes of xenon. Several thousand MOF structures have been reported, and a combination of computational and experimental tools give insight into which MOFs warrant investigation as potential adsorbents for xenon.

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**Session Classification:** Challenges of a program towards the kton scale