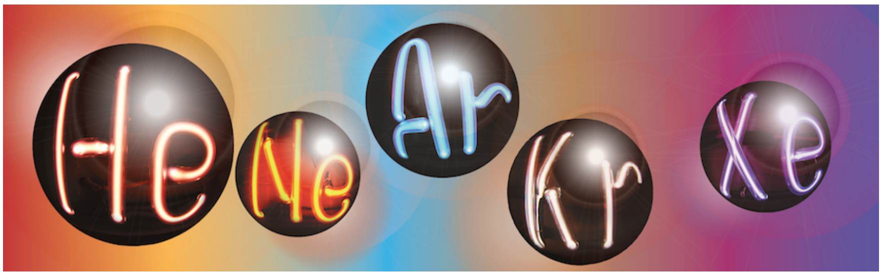

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Comparison of Oxygen Adsorbents for Large-Scale Liquid Argon Purification Using a Physics-Based Adsorption Model

The next generation of liquid argon time projection chambers, such as those employed in the Deep Underground Neutrino Experiment (DUNE), requires ultra-high purity liquid argon to ensure long electron lifetimes and optimal detector performance. Oxygen is one of the most critical electronegative contaminants, and its efficient removal during cryostat filling is essential to reduce detector commissioning time. In this work, a physics-based adsorption model is employed to compare the large-scale purification performance of the commercial BASF Cu-0226 oxygen adsorbent and an innovative reduced layered double hydroxide (R-LDH) adsorbent.

The model describes oxygen transport through the purification system by accounting for external film resistance, intraparticle pore diffusion, and Langmuir adsorption equilibrium, coupled with a transient mass balance for the cryostat. Adsorption and mass transfer parameters for both adsorbents were determined by nonlinear regression of experimental data obtained in the Liquid Argon Purification Cryostat (PuLArC) at IFGW–UNICAMP under cryogenic conditions. The calibrated models were subsequently applied to simulate the filling stage of the ProtoDUNE cryostat at CERN, enabling a direct comparison of the two materials under realistic operating conditions.

Simulation results show that, for the same adsorbent bed volume, the R-LDH material provides purification performance comparable to that of the commercial BASF adsorbent despite its significantly lower bulk density (approximately 950 kg m^{-3} compared with 2000 kg m^{-3}). Consequently, similar oxygen removal can be achieved using less than half the adsorbent mass, demonstrating the superior efficiency of the R-LDH material. Furthermore, when equal adsorbent masses are considered, the lower density of the R-LDH enables a larger adsorption bed, thereby increasing the total oxygen-capture capacity and substantially reducing the time required to achieve detector-grade liquid argon purity during cryostat filling.

These results demonstrate that experimentally calibrated adsorption models provide a robust framework for evaluating emerging purification materials at the detector scale. The superior mass efficiency of the R-LDH adsorbent highlights its potential to reduce purification costs or shorten commissioning time for future large liquid argon detectors, making it an attractive alternative to conventional commercial oxygen-getter materials.

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