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Diffusion–Model–Driven Discovery of Ferroelectrics for Photocurrent Applications

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Ferroelectric materials are vital for next-generation memory and photovoltaic technologies, yet their discovery is limited to the few known prototypes. Here, we present a design framework that integrates diffusion–model–based crystal generation with multi-fidelity screening to the discovery of ferroelectrics. Using MatterGen, we generated 12,800 candidate structures and applied a pipeline combining diverse machine-learning tools and density functional theory calculations. This process revealed two promising candidates, Ca_3P_2 and LiCdP, both insulating and switchable. The polarization value of Ca_3P_2 is 8.9 μC/cm^2 while that of LiCdP reaches as high as 144.1 μC/cm^2 which is slightly higher than that of Sc-doped AlN, one of the highest-polarization ferroelectrics reported to date. Notably, the low-temperature crystal structure of Ca_3P_2 has not been previously identified, and our study reveals a plausible candidate for this phase. In addition, HSE06 calculations yield band gaps of 1.58 and 1.13 eV for Ca_3P_2 and LiCdP, respectively, suggesting strong potential for photocurrent applications. These findings establish new promising candidates for the ferroelectric family and demonstrate the power of generative models to uncover novel functional materials.