

Supplementary Information

Crystal Habit Analysis of LiFePO_4 Microparticles by AFM and First-Principles Calculations

The X-ray diffractograms of samples A, B, C, and D corresponding to the crystal habits Wide Diamonds, Narrow Diamonds, Super-Narrow Diamonds, and Cubes are depicted in Figure S1, S2, S3, and S4, respectively. Every Figure depicts the X-ray diffraction pattern of the respective sample (top) with a respective LiFePO_4 (LFP) reference pattern (bottom). All samples show a complete overlap of all peak positions, indicating crystalline LFP.

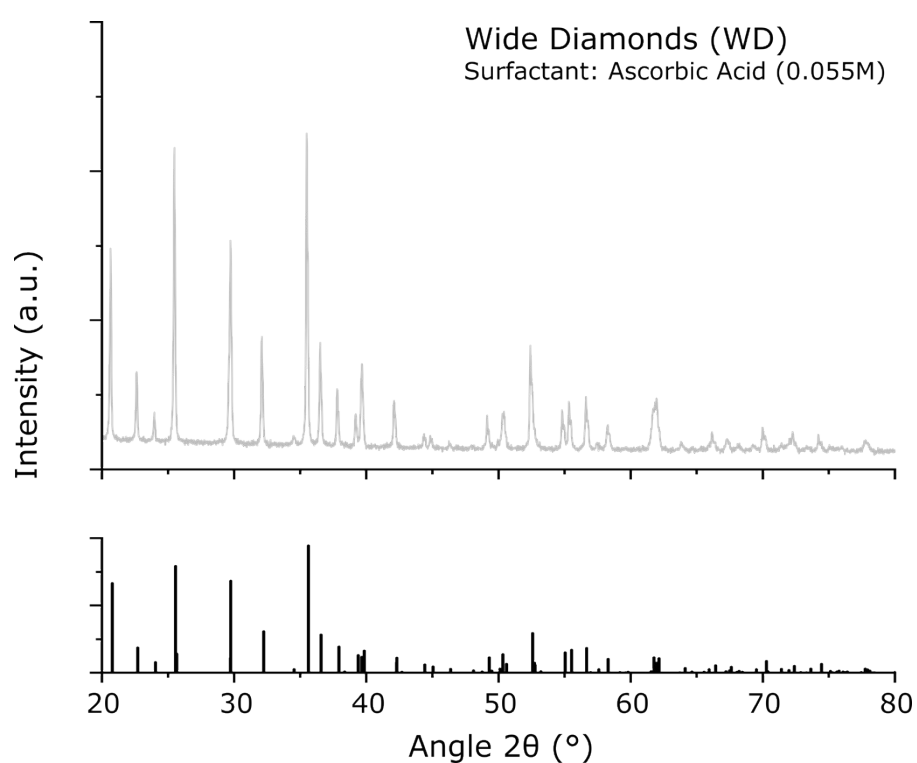


Figure S1. X-ray diffraction pattern of sample A with the wide diamond (WD) crystal habit and a reference pattern of LiFePO_4 (ICSD#92198). We find a full overlap of the peak positions, suggesting the formation of crystalline LiFePO_4 .

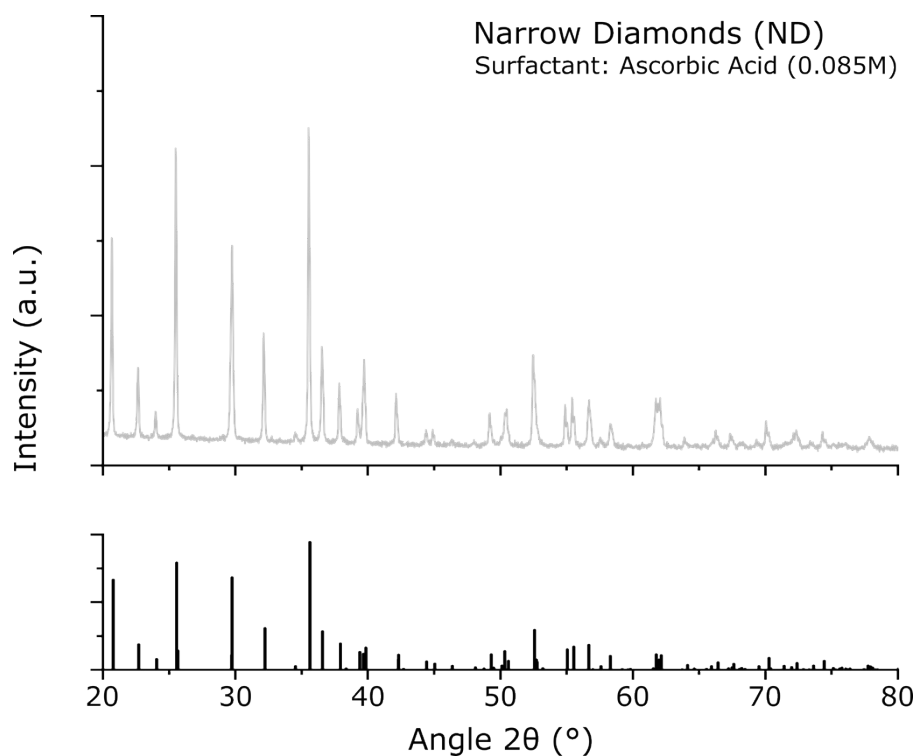


Figure S2. X-ray diffraction pattern of sample B with the narrow diamond (ND) crystal habit and a reference pattern of LiFePO_4 (ICSD#92198). We find a full overlap of the peak positions, suggesting the formation of crystalline LiFePO_4 .

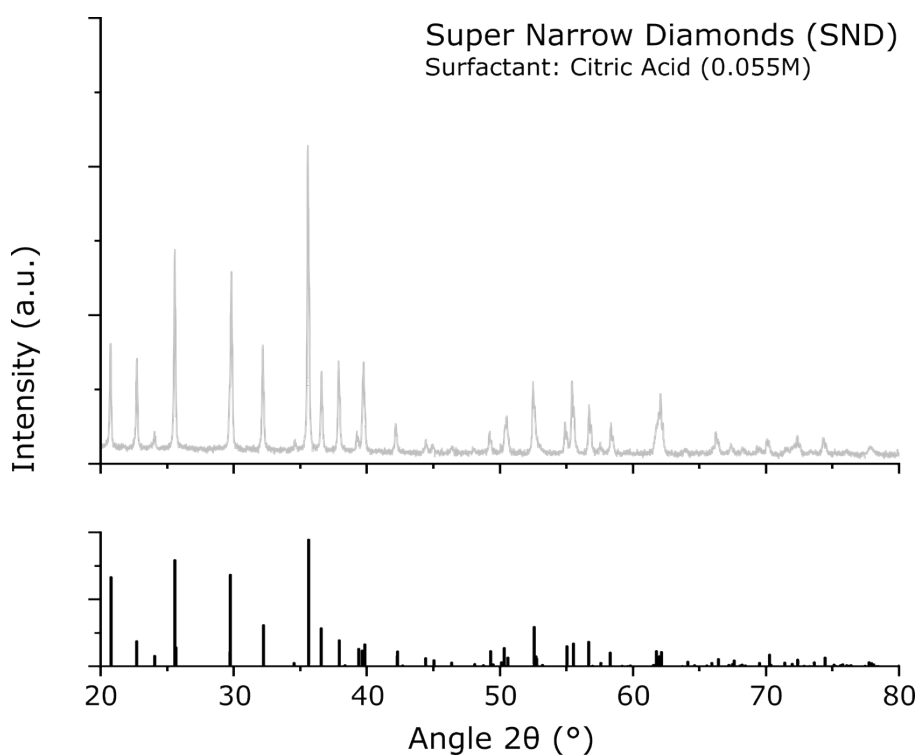


Figure S3. X-ray diffraction pattern of sample C with the super narrow diamond (SND) crystal habit and a reference pattern of LiFePO_4 (ICSD#92198). We find a full overlap of the peak positions, suggesting the formation of crystalline LiFePO_4 .

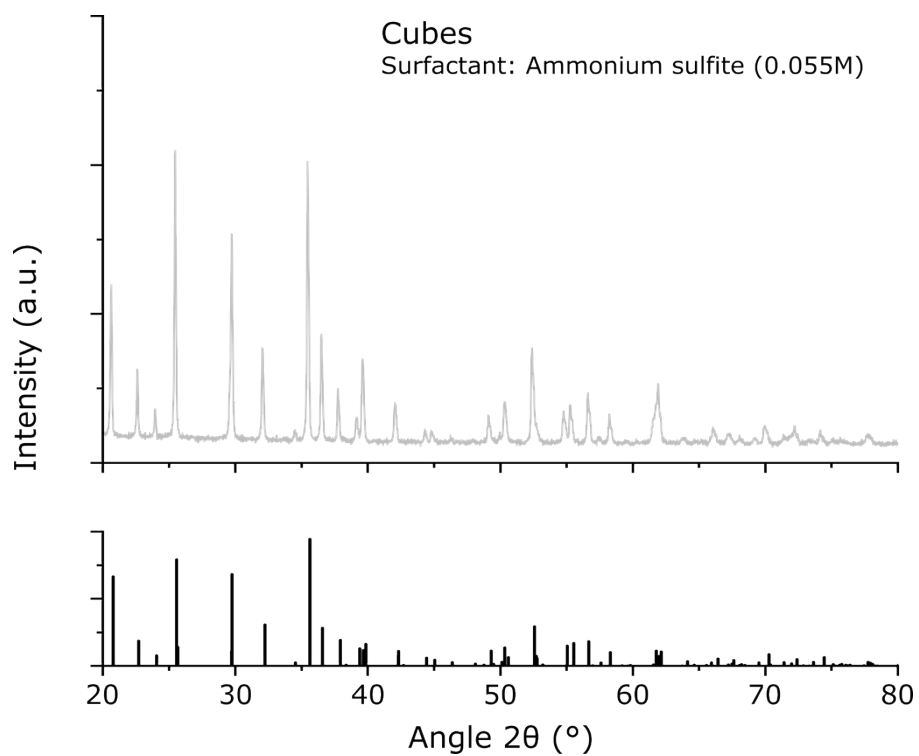


Figure S4. X-ray diffraction pattern of sample D and the Cube (CU) crystal habit and a reference pattern of LiFePO_4 (ICSD#92198). We find a full overlap of the peak positions, suggesting the formation of crystalline LiFePO_4 .