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Introduction

Polymorphism refers to the phenomenon where a single chemical compound can crystallize into two or multiple structural arrangements, each exhibiting unique physical properties despite identical molecular composition. In the context of metal organic frameworks (MOFs), polymorphism leads to structural variations, such as differing pore geometries and surface characteristics, all derived from the same chemical constituents. However, researchers have focused primarily on the pure phases of polymorphic MOFs, while intermediate-phase and mixed-phase structures have been largely overlooked due to their structural complexity and the challenges associated with their synthesis.

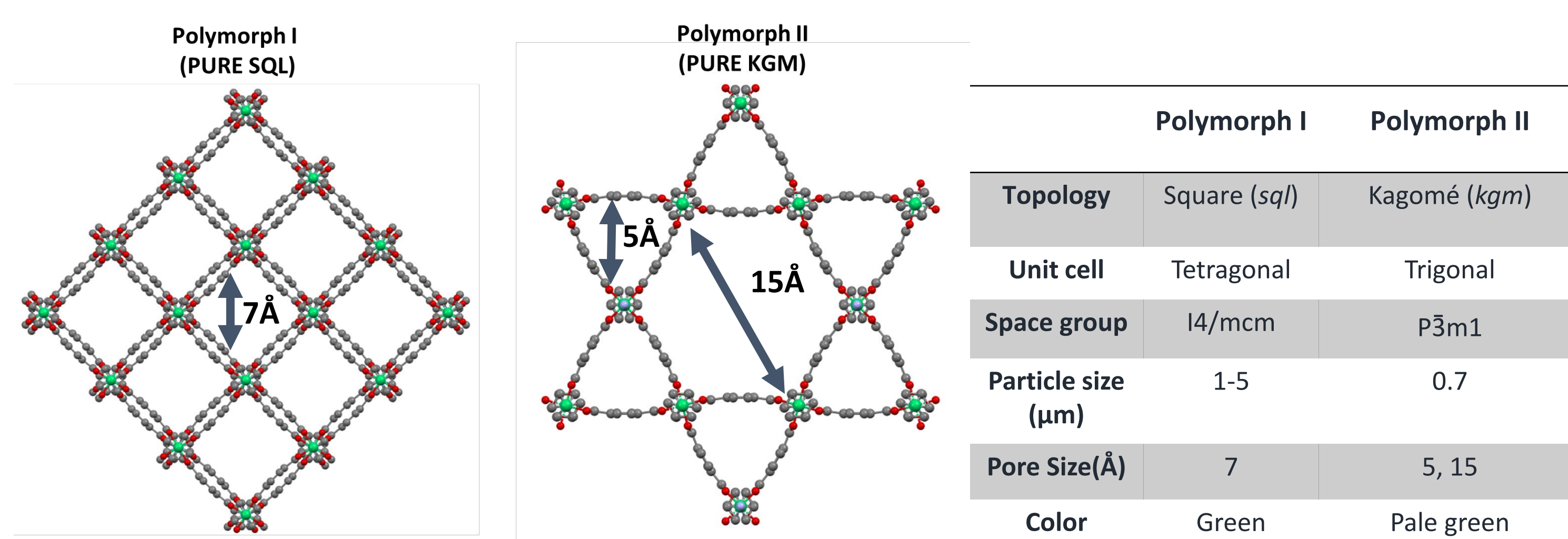
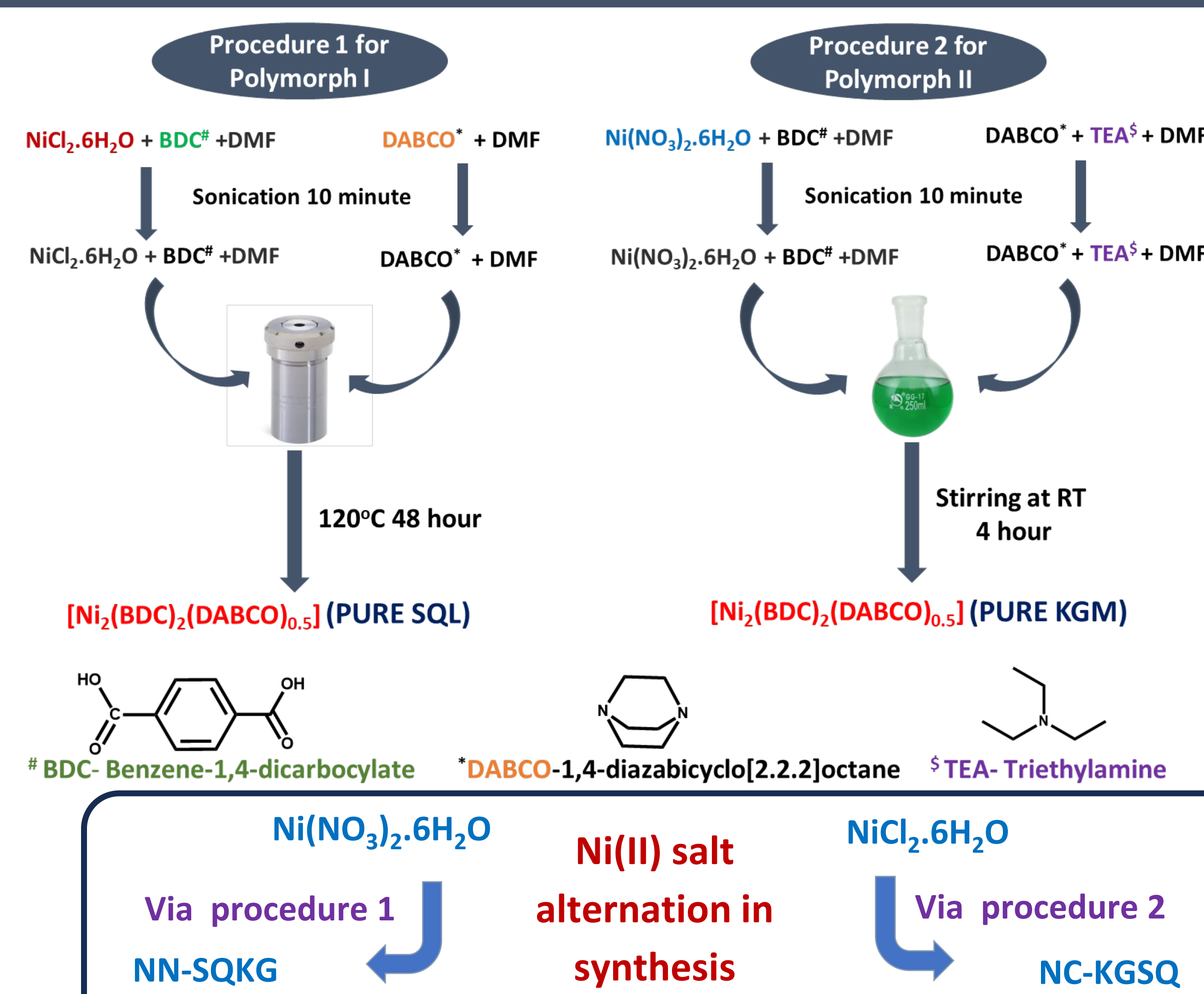


Figure 1. Two polymorphs of Ni-BDC-DABCO MOF representing *sql* and *kag* topologies.

Synthesis



Results

PXRD and SEM

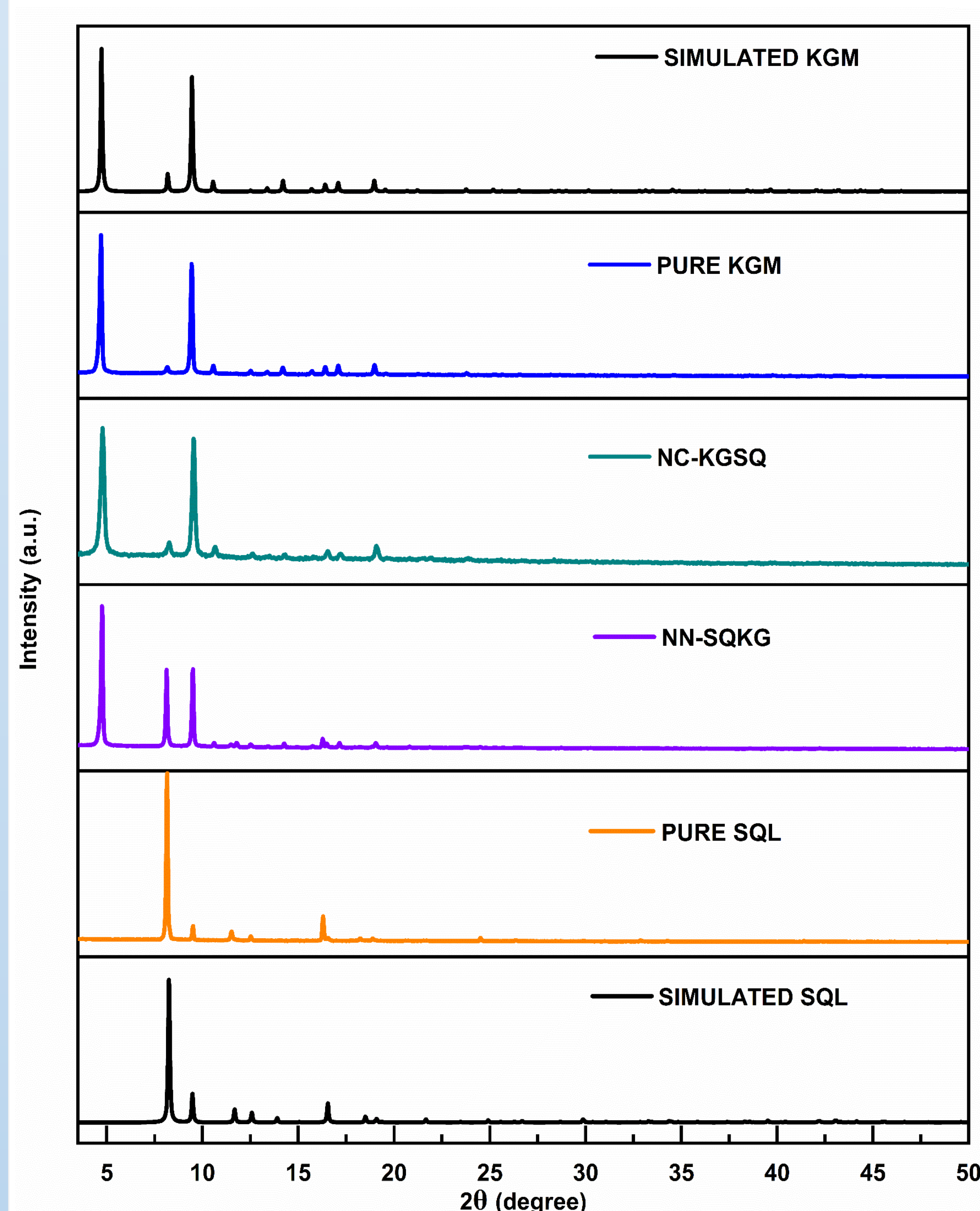


Figure 3. Comparison of PXRD patterns of PURE SQL (orange), NN-SQKG (violet), NC-KGSQ (green) & PURE KGM (blue) with the simulated patterns (top & bottom).

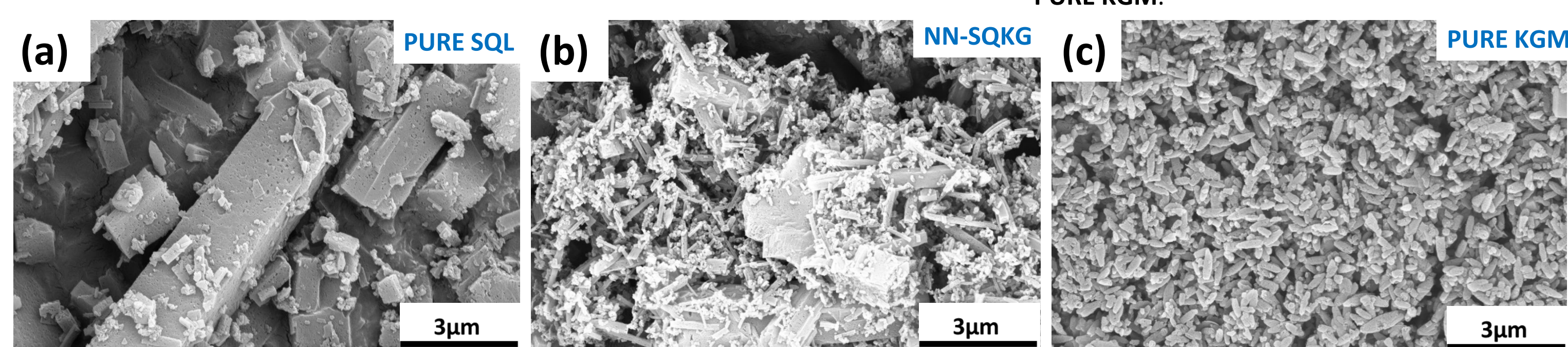


Figure 4. Scanning electron microscope (SEM) images of (a) PURE SQL (b) Mix phase sample NN-SQKG (c) PURE KGM.

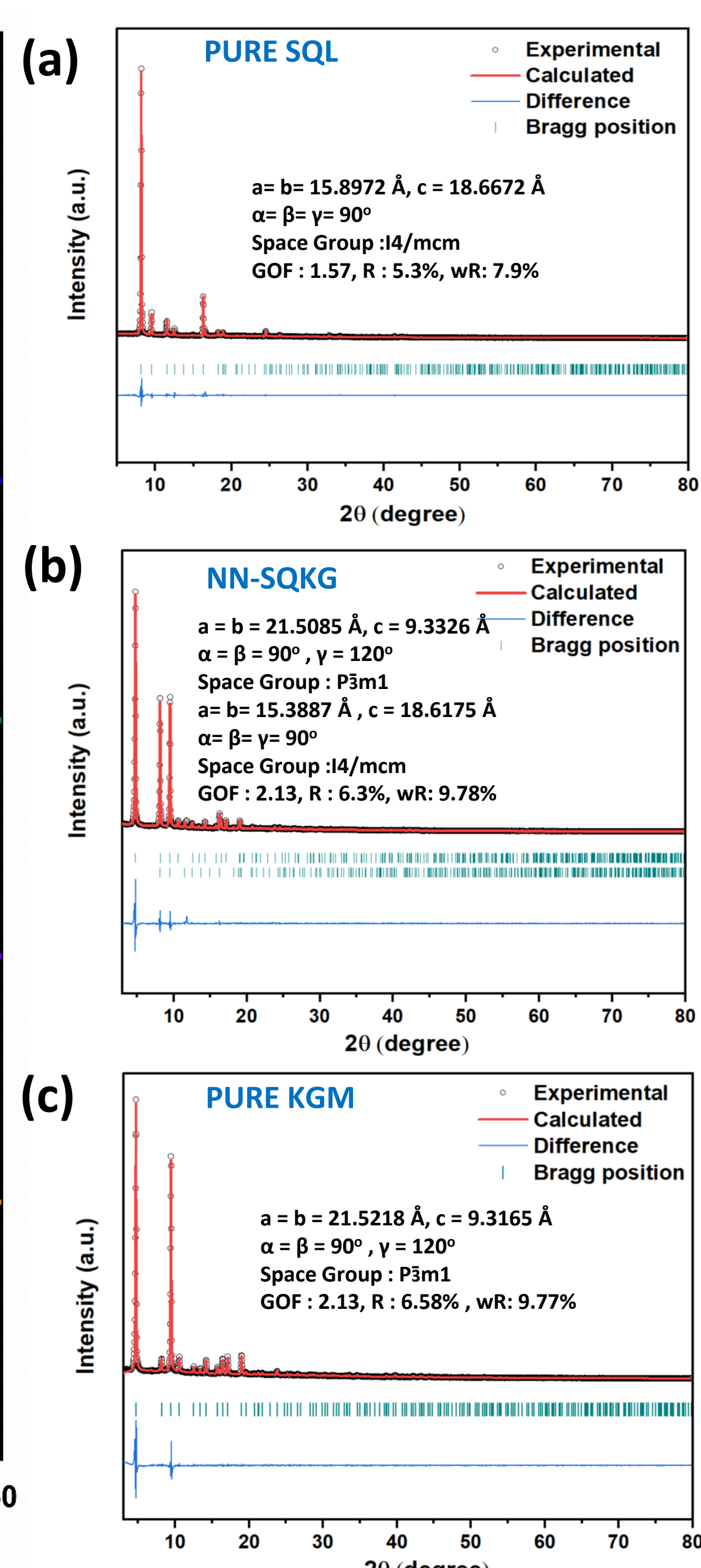


Figure 5. Le Bail fit and fitting parameters for (a) PURE SQL (b) Mix phase sample NN-SQKG (c) PURE KGM.

Gas Adsorption

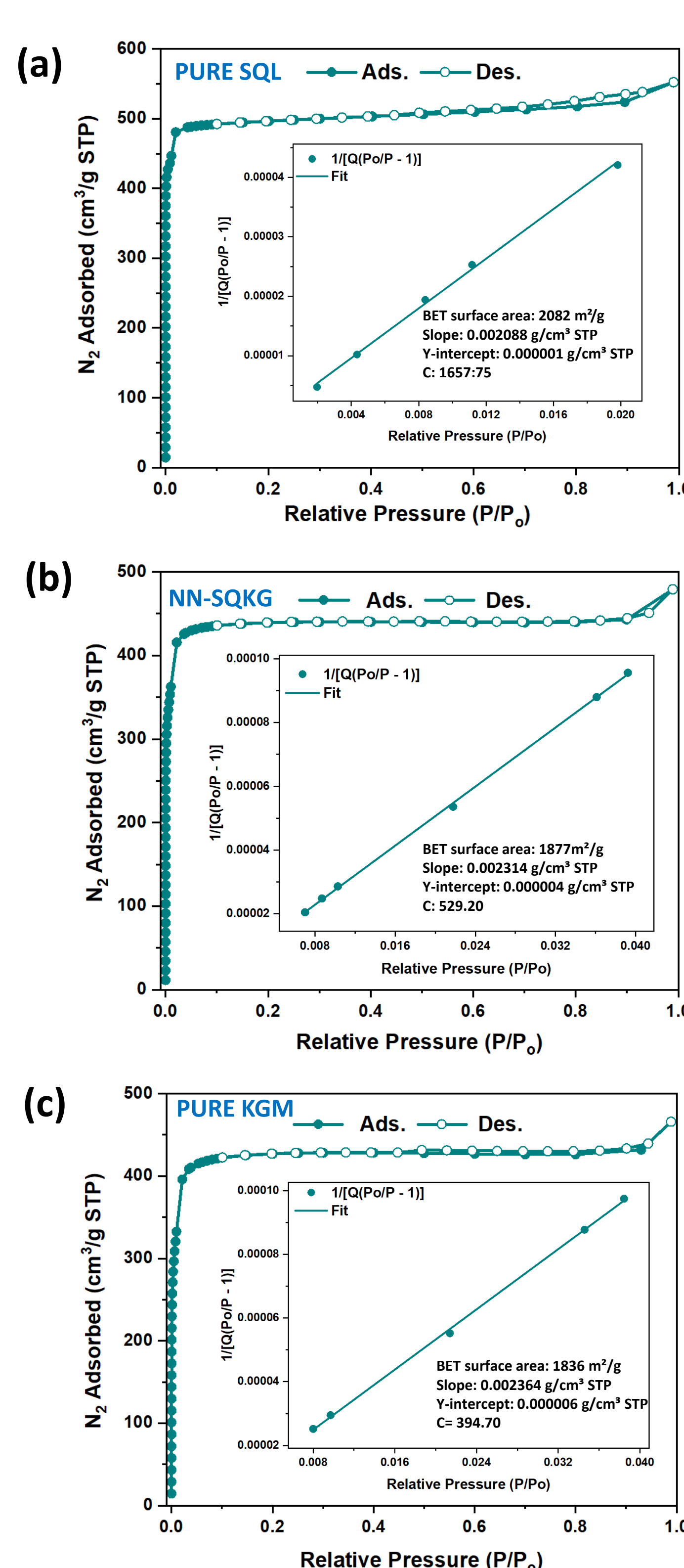


Figure 6. N_2 adsorption/desorption isotherms at 77 K (Inset: BET linear plots with fitting parameters) for (a) PURE SQL (b) Mix phase sample NN-SQKG (c) PURE KGM.

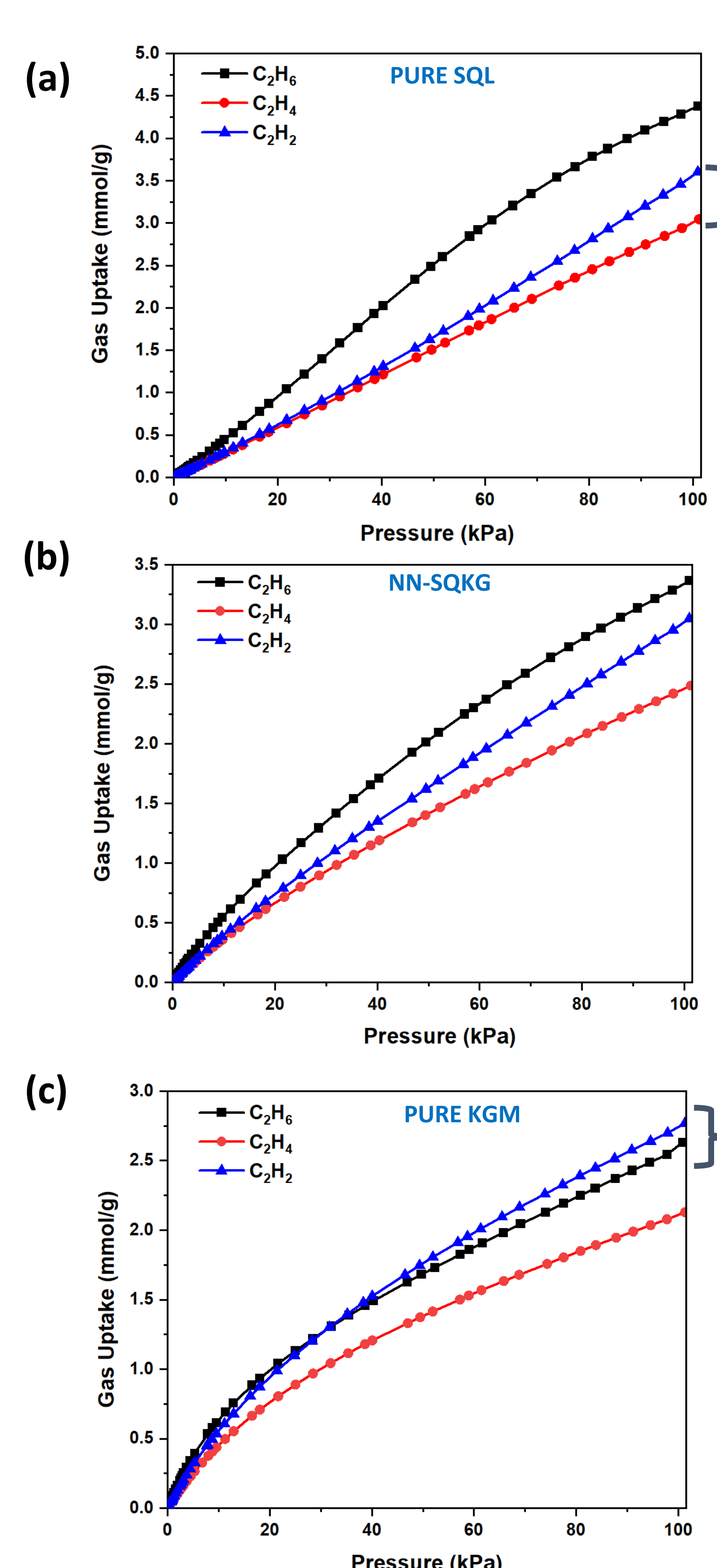


Figure 7. Adsorption isotherms of C_2H_2 (blue triangle), C_2H_4 (red circle) and C_2H_6 (black square) at 293 K for (a) PURE SQL (b) Mix phase sample NN-SQKG (c) PURE KGM.

Summary

- In this work, we revisit the polymorphism of the Ni-BDC-DABCO metal-organic framework (MOF). We synthesized and characterized four samples PURE SQL, PURE KGM, NCKGSQ, and NNSQKG under various experimental conditions.
- In addition to the well-known pure-phase polymorphs with square (*sql*) and Kagome (*kag*) topologies, we identified a mixed-phase sample, NN-SQKG, containing components of both phases.
- All samples were investigated using various structural and gas adsorption analysis techniques to explore structure-property relationships.
- Le Bail fitting was applied to the PXRD data to extract key parameters related to phase purity.
- Single-gas adsorption measurements demonstrated the promising potential of the mixed-phase sample NN-SQKG for tuning the uptake of C_2 gases. Further studies on diffusion rates are planned to evaluate the application of the mixed-phase sample in membrane-based gas separation.

References

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Acknowledgement



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