

Characterisation of Na⁺ dynamics in $\text{Na}_{3-2x}\text{Mg}_x\text{PO}_4$

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Solid-state ionic conductors have been increasingly investigated as an alternative to liquid electrolytes in solid state sodium ion batteries. Whilst much progress has been made in the design and development of promising candidate materials, their complex structures and difficulties in probing dynamics beyond the bulk picture has meant that understanding the mechanisms involved in Na⁺ diffusion remains a challenge. Quasi-elastic neutron spectroscopy (QENS) is one avenue which provides an opportunity to gain insight into these mechanisms at the atomic level.

This work focuses on characterising sodium-ion self-diffusion using QENS in Mg²⁺ stabilised $\text{Na}_{3-2x}\text{PO}_4$. From a dynamics perspective, $\text{Na}_{3-2x}\text{PO}_4$ is of interest since its structure features multiple inequivalent sodium sites, forming non-Bravais sublattices.[1] Since it cannot be known a priori which site(s) are involved in the diffusion, the standard approach[2] which is used to model the QENS dynamic scattering function $S(Q, \omega)$ in similar systems does not generally describe the diffusion mechanisms at play. Consequently, we have modelled the $S(Q, \omega)$ through the construction of a matrix to account for all possible jumps within the material by solving the corresponding eigenvalue problem.[3,4] Here, we present the insight that this approach provides on details of the possible Na⁺ diffusion mechanisms, including diffusion paths and relaxation times.

[1] D. Wilmer and J. Combet, Chemical Physics 292 (2), 143-152 (2003).

[2] C. T. Chudley and R. J. Elliott, Proceedings of the Physical Society 77 (2), 353 (1961).

[3] J. M. Rowe, K. Sköld, H. E. Flotow and J. J. Rush, Journal of Physics and Chemistry of Solids 32 (1), 41-54 (1971).

[4] O. G. Randl, B. Sepiol, G. Vogl, R. Feldwisch and K. Schroeder, Physical Review B 49 (13), 8768-8773 (1994).

Level of Expertise

Student

Do you wish to take part in the poster slam

No

Travel Funding

No

Speakers Gender

Female

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