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Investigation of ionic transport in sodium scandium phosphate (NSP) and related compounds KAUSTUBH BHAT, STEFAN BLÜGEL, HANS LUSTFELD, Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — Sodium ionic conductors offer significant advantages for application in large scale energy storage systems. In this study, we investigate the different pathways available for sodium ion conduction in NSP and calculate energy barriers for ionic transport using Density Functional Theory (DFT) and the Nudged Elastic Band Method [2]. We identify the structural parameters that reduce the energy barrier, by calculating the influence of positive and negative external pressure on the energy barrier [3]. Lattice strain can be introduced by cation or anion substitution within the NASICON structure. We substitute the scandium atom with other trivalent atoms such as aluminium and yttrium, and calculate the resulting energy barriers. Sodium thiophosphate (Na_3PS_4) has previously shown about two orders of magnitude higher ionic conductivity than sodium phosphate (Na_3PO_4) [4]. We investigate the effect of substituting oxygen with sulphur in NSP. We acknowledge discussions with our experimental colleagues F. Tietz and M. Guin toward this work. [1] Hong, MRB **11**, 173-182 (1976). [2] Henkelman et al. JCP **113**, 9901-9904 (2000). [3] Hirschfeld et al. PRB **84**, 224308 (2011). [4] Hayashi et al. Nat. Comm. **3**, 856 (2012).

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