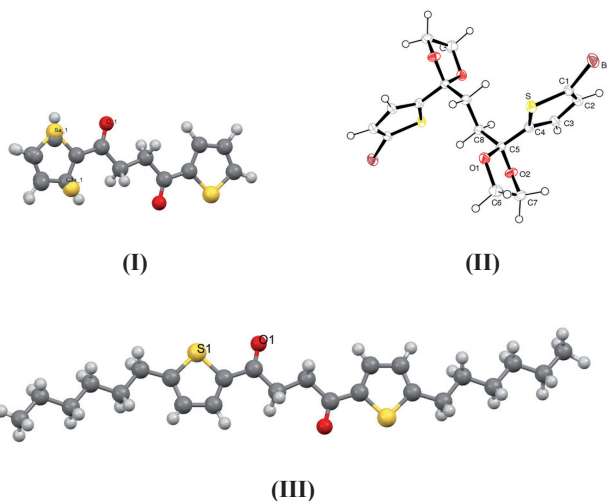


position [2]. In this type of molecules, it is observed, however, that the thiophene ring often shows a disorder [3] even at low temperature, if the adjacent environment allows for free rotation around a single bond. Thus the structural analysis is extremely important for substitution and chain extension at the required position to obtain the required electrochemical efficiency. The experimental analysis of the electronic environment is also desirable to obtain the optimum efficiency of the target molecule. In the meeting, three different representative cases of thiophene based compounds will be presented. The case of *1,4-bis (2-thienyl) butane-1,4-dione* (I), for which the modelling is done for the disordered thienyl group. Secondly, the case of *2, 2'-(1, 2-ethanediy) bis [2-(5-bromo-2-thienyl)-1, 3-Dioxolane* (II), for which the electron density parameters have been transferred from the ELMAM2 database [4] and lastly, the case of *1,4-bis (5-hexyl-2-thienyl) butane-1,4-dion* (III), whose experimental electron density analysis is underway using MoPro software [5].



[1] M. Grätzel, *Nature*. **2001**, *414*, 338. [2] C. Roux, J.-Y. Bergeron, M. Leclerc, *Macromo. Chem.* **1993**, *194*, 868-877. [3] S. Wang, F. Brisse, F.B. Gariéy, A.D. Bouillud, M. Leclerc, *Acta. Cryst.* **1998**, *C54*, 553-555. [4] S. Domagala, P.M. Munshi, M. Ahmed, B. Guillot, C. Jelsch, *Acta. Cryst.* **2011**, *B67*, 63-78. [5] C. elsch, B. Guillot, A. Lagoutte, C. Lecomte, *J. Appl. Cryst.* **2005**, *38*, 38-54.

**Keywords:** solar cells, thiophenes, electron density

### MS39.P02

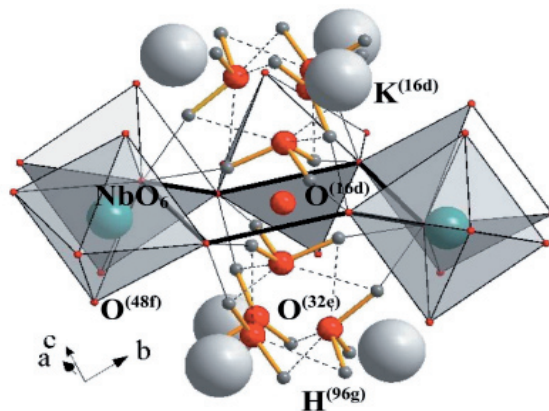
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**The exotic ions arrangement in the pyrochlore -type framework of protonic conductor  $K_{0.88}Nb_2O_7.58H_{4.28}$  for intermediate temperature PSOFCS**

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According to single-crystal, synchrotron powder X-ray diffraction and neutron powder diffraction studies, the novel pyrochlore-type compound contains the water molecules located in 32e sites, the hydroxide ions and potassium ions are located in 16d sites with a significant amount of 'free' protons in 96g sites corresponding to the structural formula  $K_{0.88}(OH)_{0.54}H_{1.66}(H_2O)_{1.04}Nb_2O_6$ . The total weight loss at temperatures up to 773 K is limited to about 8%, suggesting the oxygen escape from 48f sites can be excluded and 'free' protons must be kept in the structure. The bulk conductivity in ambient air reaches the plateau at  $10^{-2} S \cdot cm^{-1}$  for 623 K. Owing to the wide stability range and resistance to water solubility, the compound can be considered as a

candidate to fill the gap for intermediate temperature solid-oxide fuel-cell applications materials. Even more hydrogen-containing materials are prepared with ion exchange for protons.



*The protonic sites in hydrothermally grown  $K_{0.88}Nb_2O_7.58H_{4.28}$  as extracted from neutron powder diffraction data.*

[1] O. Smirnova, N. Kumada, T. Takei, Y. Yonesaki, M. Yashima, N. Kinomura. *Acta Cryst.* **2010**, *B66*, 594-602.

**Keywords:** protonic conductor, intermediate temperature SOFCs, powder diffraction

### MS39.P03

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**Rationalising the molecular origins of dyes used in dye sensitized solar cells**

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The dye sensitized solar cell (DSC) has been at the forefront of worldwide research since the pioneering work of O'Regan and Grätzel [1] showing that these devices can achieve a power conversion efficiency of over 11%. One of the key aspects controlling the performance of the DSC is the molecular nature of the dye used. However, even after two decades of study, one of the first ever produced dyes for DSC's (N719) still provides record efficiencies. This is puzzling as the DSC field is so driven by economics and Ruthenium, which is contained in N719, is a rare transition metal making it relatively expensive.

We have used X-ray diffraction and accompanying statistical analysis to compare three Ruthenium based dyes and one Iron based dye which are structurally similar to N719 in order to elucidate why it is still one of the best performing dyes to date. Iron and Ruthenium lie in the same group of the periodic table. Consequently the Iron based dye has been considered as a cheaper alternative to Ruthenium based dyes despite affording reduced efficiency.

Our X-ray diffraction studies concentrate on a Ruthenium dye and an Iron dye that have the same principal molecular structure but different counter ions. We also looked at the structural differences of the previously mentioned Ruthenium dye with and without carboxylate groups attached. These structures were all compared to that of N719 both structurally and spectroscopically.

The Cambridge Structural Database (CSD) was then employed