

**MS12-05** **Molecularbasis of cholera blood group dependence** Julie Elisabeth Heggelund,<sup>a</sup> Espen Haugen,<sup>a</sup> Birgitte Lygren,<sup>b</sup> Alasdair Mackenzie,<sup>a</sup> Åsa Holmner,<sup>ac</sup> Francesca Vasile,<sup>d</sup> José Reina,<sup>d</sup> Anna Bernardi<sup>d</sup>, UteKrengel,<sup>a</sup> <sup>a</sup>University of Oslo, Department of Chemistry, Norway, <sup>b</sup>University of Oslo, Biotechnology Center of Oslo and NCMM, Norway, <sup>c</sup>Umeå University, Radiation Sciences - Biomedical Engineering R&D, Sweden, <sup>d</sup>Universita' degli Studi di Milano, Dipartimento di Chimica, Italy  
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Cholera is a serious diarrhoeal disease that claims hundreds of thousands of deaths every year. The disease is known to be strongly blood-group dependent, with blood group O individuals experiencing increased risk of severe symptoms, but the molecular basis of this blood-group dependence has remained unknown. Since blood group O individuals are not more likely to be infected, the main suspect is major virulence factor of *Vibrio cholerae*, the Cholera toxin (CT). Here, we present results showing that both El Tor and classical cholera toxin B-pentamers indeed bind blood group determinants (with equal affinities), using Surface Plasmon Resonance and NMR spectroscopy [1]. Taken together with our previous crystallographic data for CTB variants in complex with a blood group A analog [2,3], a picture emerges as to the molecular basis of cholera blood group dependence.

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**MS13-01** **Local structure investigation of clean energy materials through pair distribution function analysis.** Lorenzo Malavasi,<sup>a</sup> <sup>a</sup>Department of Chemistry and INSTM, University of Pavia, Italy  
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The knowledge of the structural properties of crystalline materials is one of the most essential piece of information we need to obtain in order to make reliable correlations with physical properties, especially in functional materials. Traditional crystallographic methods based on single crystal and powder X-ray and neutron diffraction are the preferred methods to look at the *average* structure of a crystalline material. The progress in the synthesis of complex materials with enhanced properties showed that a full understanding of their structural features may not be obtained with the use of diffraction alone. Materials which are not fully periodic, like nanocrystalline or highly disordered compounds, require new experimental approaches that can tackle the structural issues to a high degree of accuracy [1]. In this context, materials for clean energy applications, such as highly defective oxides and nanocrystalline compounds (which are becoming extremely popular in this area) for a range of applications (solid oxide fuel cells, lithium batteries, hydrogen storage materials) need to be treated with a new approach that could open the possibility to study their *local* structure and unveil structural features which cannot be assessed with traditional crystallographic methods. This approach centres around the *atomic pair distribution* (PDF) technique.

In the past, PDF analysis has been used for many years for studying materials with no long-range order such as liquids and glasses. The advent of high power X-ray and neutron sources allowed to apply the PDF analysis to the investigation of crystalline materials. The essential difference with respect to the traditional crystallographic methods, which make use of the structural information contained in the Bragg peaks, is the use of the *total scattering* coming from the sample which include the Bragg and diffuse scattering [2]. This part of the sample scattering become more and more important as the long-range order breaks on the atomic-scale and the PDF technique allow to reveal the short and intermediate order of the material regardless of the degree of disorder.

In this presentation we are going to give first a concise description of the PDF technique and then an overview about the successful application of total scattering methods to the investigation of crystalline materials for clean energy applications. We should stress that, with respect to other classes of materials, the application of the PDF technique to materials for energetics is more recent. However, such new approach already showed its power in order to provide information at the atomic scale level that are essential to give new insights, for example, about the mechanisms involved in the carrier motion, study the defects structure and find correlations between different crystal structure of a material [3-8]. Examples will cover new oxide ion conductors such as La<sub>2</sub>Mo<sub>2</sub>O<sub>9</sub>, Ge-apatites, Ga-based melilites and Ba-indates.

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