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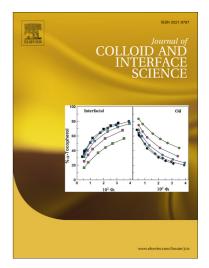
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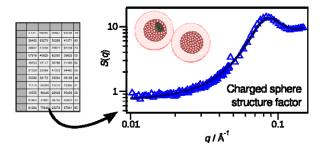
ACCEPTED MANUSCRIPT

A simple and accurate method for calculation of the structure factor of interacting charged spheres

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Calculation of the structure factor of a system of interacting charged spheres based on the Ginoza solution of the Ornstein-Zernike equation has been developed and implemented on a stand-alone spreadsheet. This facilitates direct interactive numerical and graphical comparisons between experimental structure factors with the pioneering theoretical model of Hayter-Penfold that uses the Hansen-Hayter renormalisation correction. The method is used to fit example experimental structure factors obtained from the small-angle neutron scattering of a well-characterised charged micelle system, demonstrating that this implementation, available in the Supplementary Information, gives identical results to the Hayter-Penfold-Hansen approach for the structure factor, S(q) and provides direct access to the pair correlation function, g(r). Additionally, the intermediate calculations and outputs can be readily accessed and modified within the familiar spreadsheet environment, along with information on the normalisation procedure.



Graphical abstract

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