Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Charge distribution from SKPM images

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$V_{\text{SKPM}}^{\text{Charge}}$ from a known charge distribution

Although it is not the final aim of this work, a useful application of the proposed FFT–based method is to obtain the expected V_{SKPM} image from a known charge distribution. Using the equation

$$V_{\text{SKPM}}^{\text{Charge}}(x, y, d_0) = \text{IFT}(q(\mathbf{k}_{ij})V_{\text{SKPM}}^{\text{point}}(\mathbf{k}_{ij})) \tag{1}$$

the $V_{\text{SKPM}}^{\text{Charge}}(x, y, d_0)$ image is easily computed if $V_{\text{SKPM}}^{\text{point}}(x, y, d_0)$ is properly modelled for a specific system. This may reduce enormously the numerical effort since we only need the V_{SKPM} image of one "point–charge", instead of taking into account a large number of charges. Figure S1 shows an example of this procedure. Comparing the $V_{\text{SKPM}}^{\text{Charge}}$ images obtained with the FFT–based and the image charges–based method for the same charge distribution, we can see that they are essentially the same except in the image borders, which is due to the different boundary conditions used in the calculation.

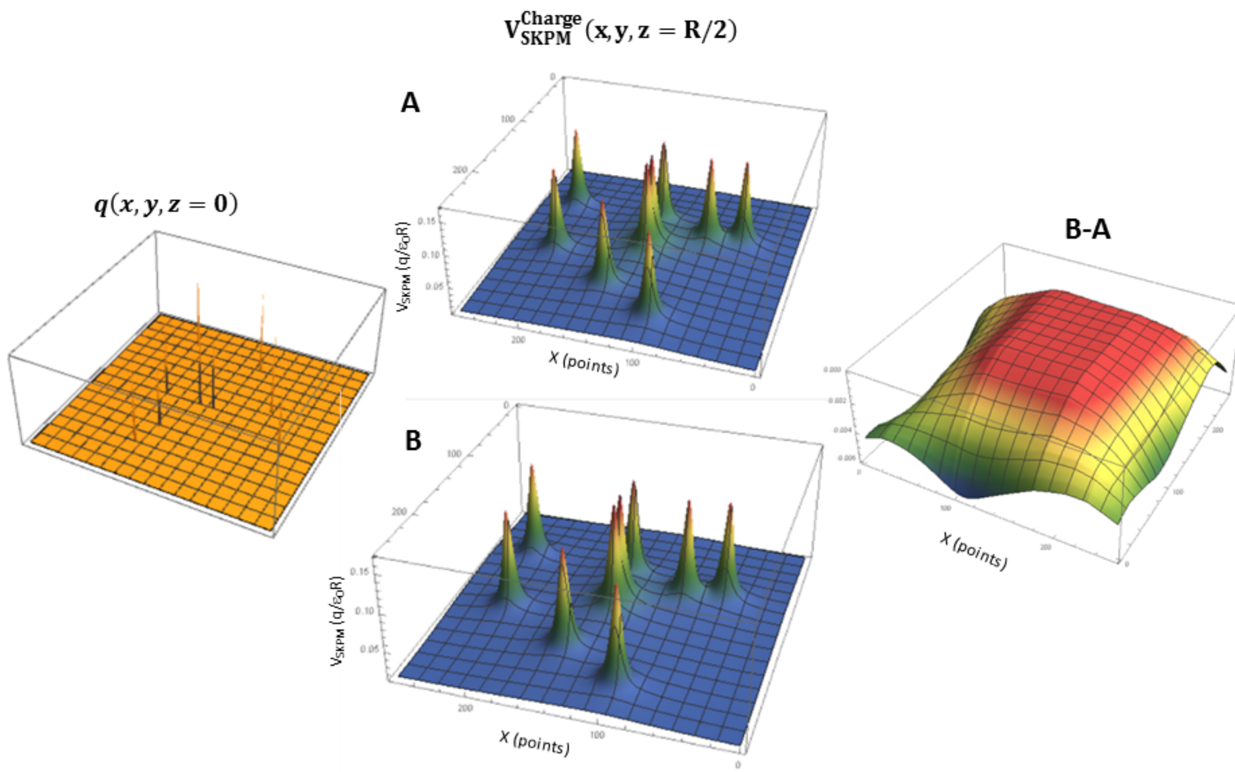

Figure S1: $V_{\text{SKPM}}^{\text{Charge}}$ images obtained with A) FTT–based method and B) image charges–based method for an arbitrary positive unitary ($+e$) point charges distribution (left panel). The right panel shows the difference between B and A. Images size is 256×256 points and $\varepsilon_r = 4.1$.

Border discontinuities removal

As we have discussed in the main text, in V_{SKPM} images the use of periodic boundary conditions introduces spurious charge discontinuities at the image edges. To overcome this problem, a possible solution is to smooth the V_{SKPM} steps at the borders. To do so, we proceed as follows: in order to reproduce the periodic boundary conditions, we applied a shift function to the original V_{SKPM} image, exchanging the four image quadrants. Then, we apply a Gaussian filter–mask (circular mask filtered using a Gaussian filter) to the central cross of the image. As shown in Figure S2, this smooths the discontinuities at the edges. Finally, we reconstruct the "edge smoothed" image to use it as the V_{SKPM} image input for the charge calculation. The width of the central cross and the parameters of the filter (smoothed points) should be tuned depending on the original images.

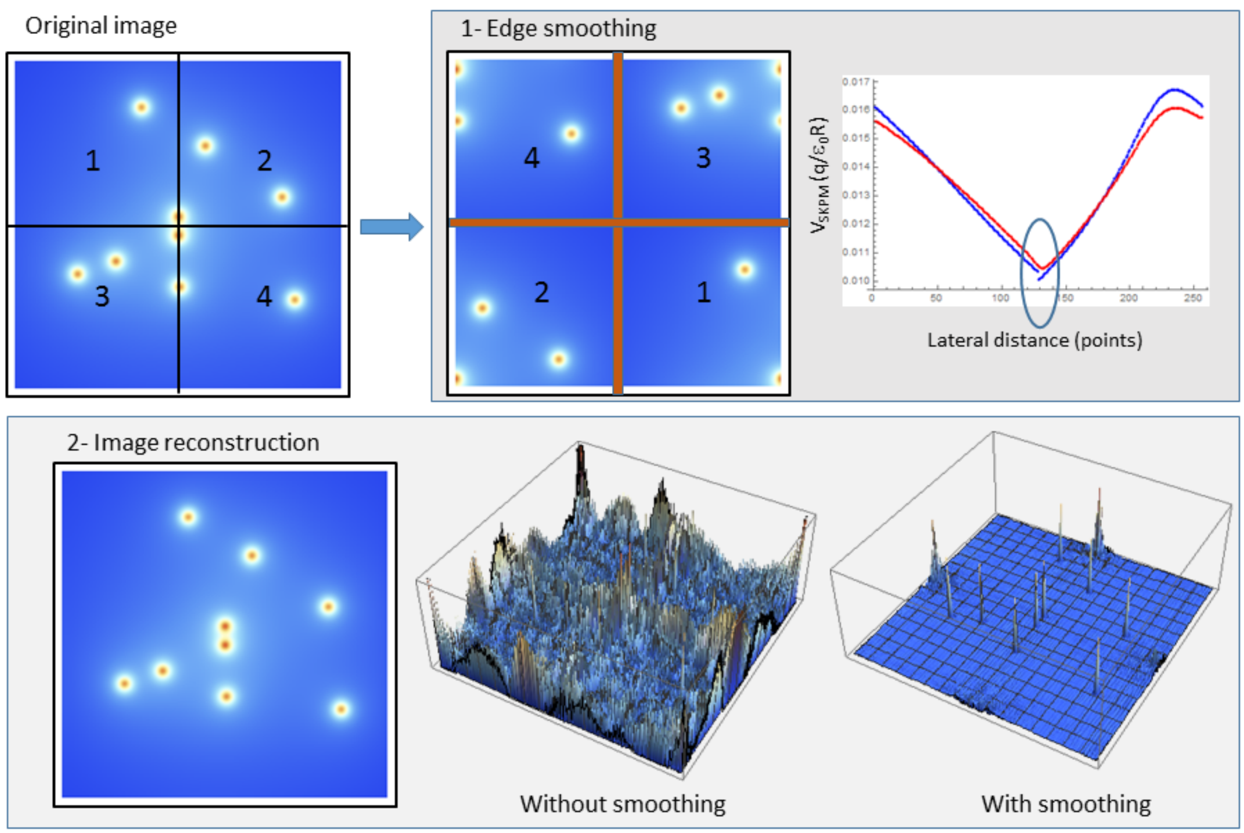

Figure S2: Step by step procedure to smooth the discontinuities at the border of the image. In the bottom panel the $q(x, y)$ images obtained from the original V_{SKPM} without and with edge discontinuities removal are compared.

Charge domains on PMMA surface: selection of the radius r_k

Figure S3 shows the $q(x, y)$ obtained from the forward and backward experimental V_{SKPM} images acquired on PMMA for different cut–off filter radii. The larger the radii, the lateral resolution increases, while the cross–correlation between forward and backward decreases due to the noise spurious contribution. We have set r_k in order to have the larger lateral resolution with a high cross–correlation ($r = 11$ points, cross–correlation $= 0.9$).

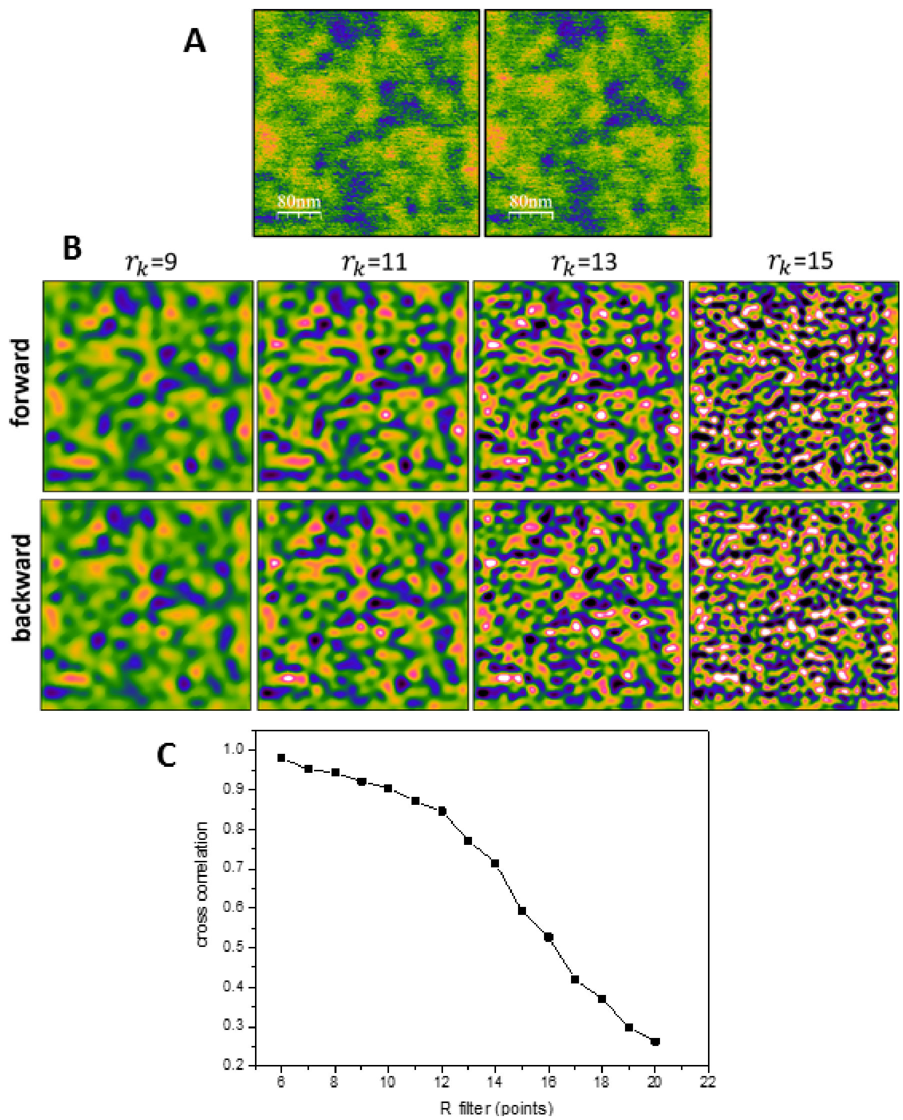

Figure S3: A) Forward and backward V_{SKPM} images acquired on PMMA. B) Forward and backward $q(x, y)$ obtained from A) for different cut–off filter radii. C) Cross–correlation function of the forward and backward $q(x, y)$ images as a function of the cut–off filter radii.