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**Supporting information for article:**

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**Michał Kamiński, Karolina Jurkiewicz, Andrzej Burian and Aleksander Bródka**

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In order to consider effects of the instrumental *Q*-resolution the NIST Si 640e standard was measured under the same experimental conditions as the gold nanoparticles. A comparison shown in Figure S1 indicates that the instrumental broadening function, represented by the (111) peak of the standard, has width significantly narrower than those of the sample peaks.

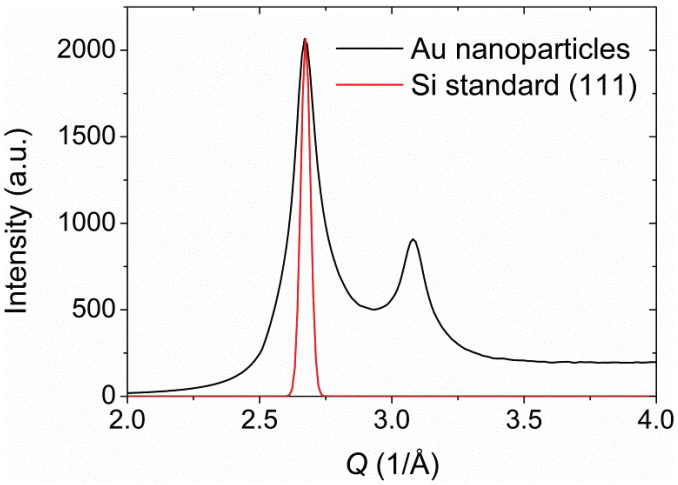


**Figure S1** The measured intensity profiles of the first two diffraction peaks of the Au NPs and the (111) peak of the NIST Si 640e standard. The Si (111) peak is shifted to the position of the first Au NPs peak and scaled to its maximum.

Effects of the *Q*-resolution on the calculated structure factors and PDFs are illustrated in Figures S2 and S3. The structure factors and the PDFs calculated before and after convoluting with instrumental broadening function for the considered models differs only slightly, indicating that the *Q*-resolution of the used instrument does not lead to significant changes both in reciprocal and real spaces. It is especially noticeable for higher *Q*-range where the peaks are more broadened.

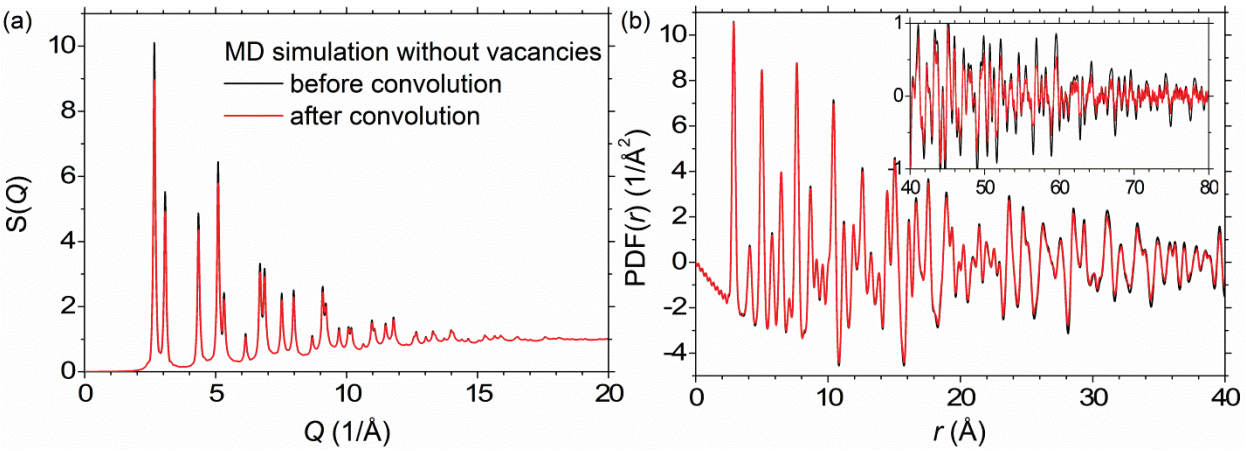


**Figure S2** Comparison of the structure factors (a) and the PDFs (b) for the model without vacancies before and after convolution of the calculated intensities with the instrumental resolution function.

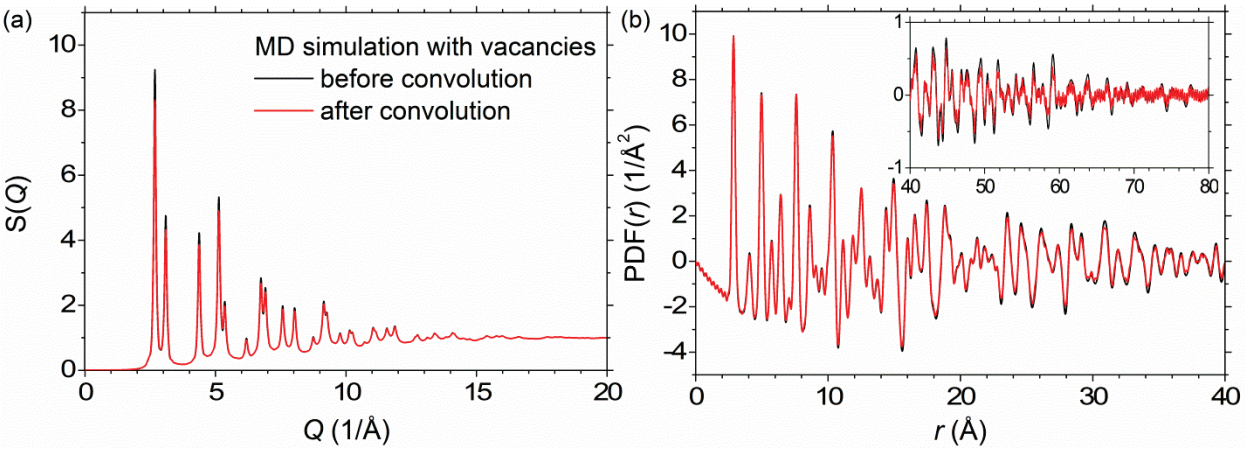


**Figure S3** Comparison of the structure factors (a) and the PDFs (b) for the model with vacancies before and after convolution of the calculated intensities with the instrumental resolution function.

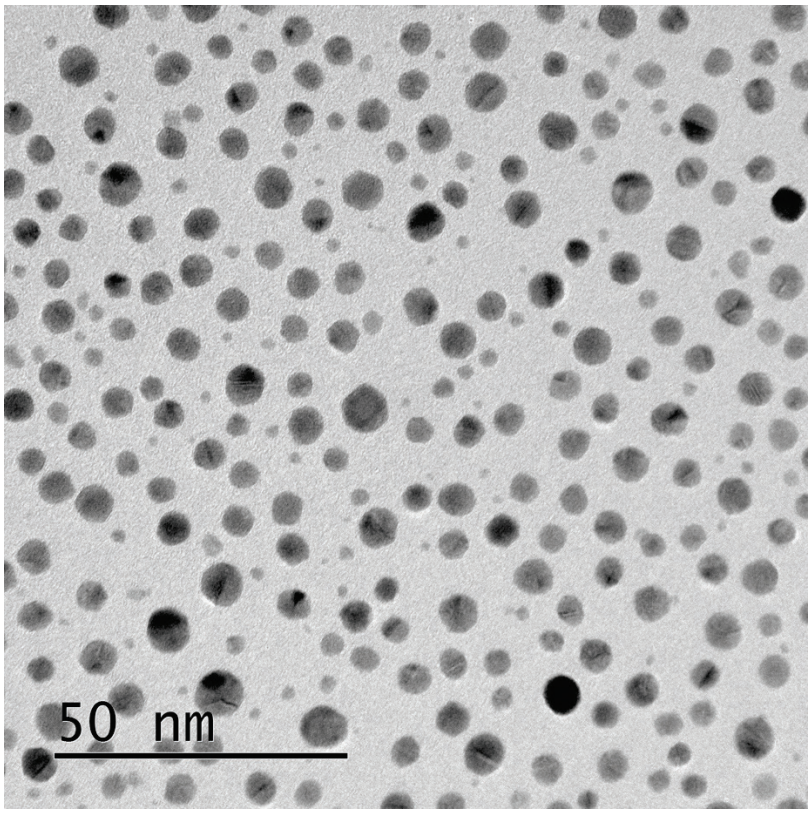


**Figure S4**. Transmission electron microscopy image of the investigated gold nanoparticles.

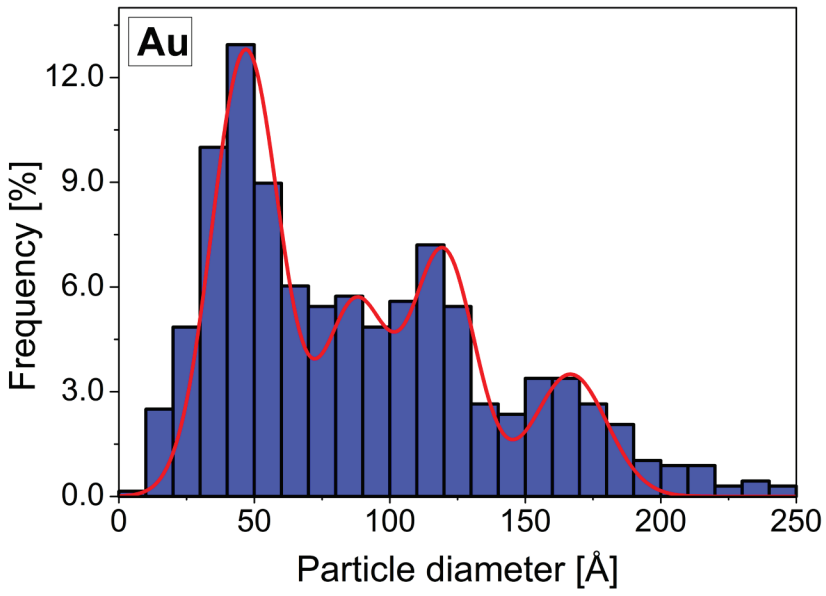


**Figure S5**. The diameter distribution of the gold nanoparticles (Jurkiewicz *et al*. 2018).

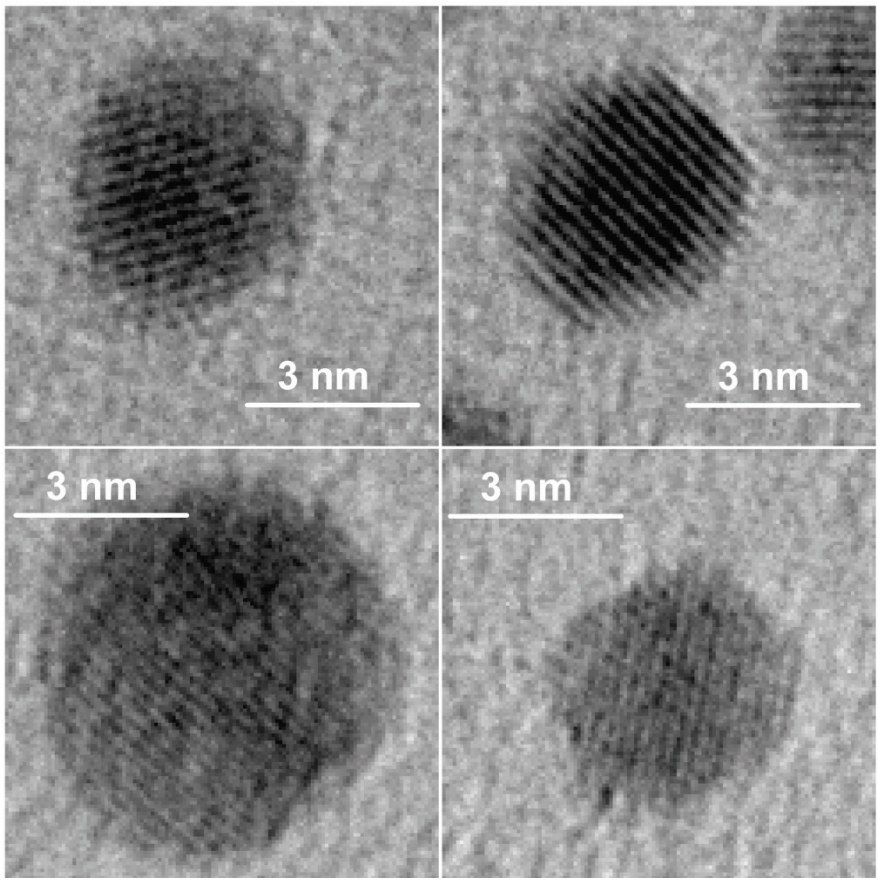


**Figure S6.** Enlarged fragments of the transmission electron microscopy image shown in figure S4.