Electronic Supplementary Material (ESI) for Nanoscale.

SUPPLEMENTARY MATERIAL

Electronic properties of $MoSe_2$ nanowrinkles

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S1. UNIT CELLS AND BRILLOUIN ZONES

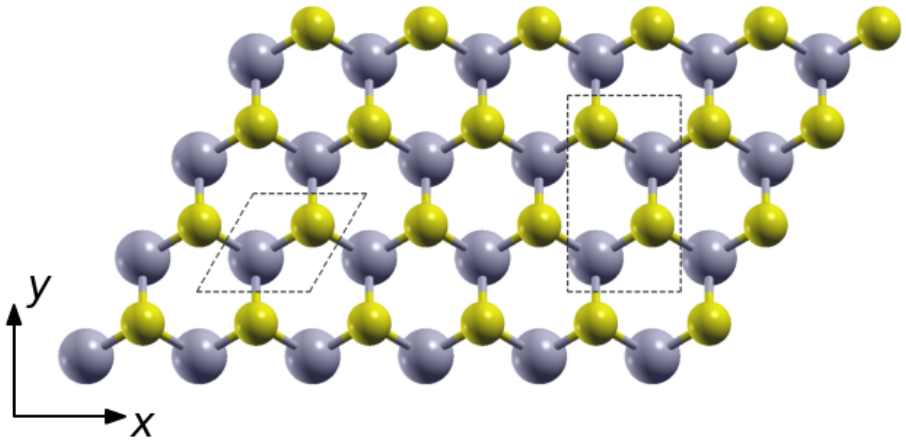

FIG. S1. Ball-and-stick representation of the $MoSe_2$ monolayer, with hexagonal and orthogonal unit cells highlighted by dashed lines. Mo atoms are shown in grey and Se atoms in yellow. The image was visualized using XCrySDen [1].

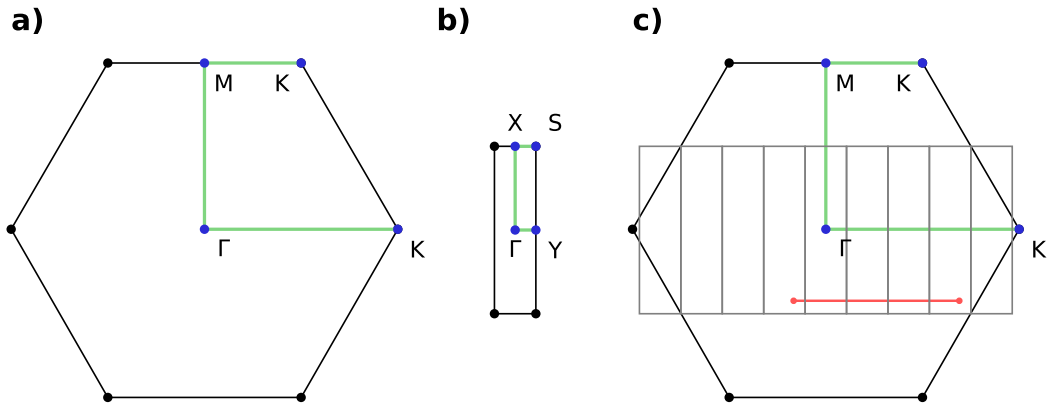

FIG. S2. Schematic representation of the Brillouin zone (BZ) associated with a) the hexagonal unit cell of pristine $MoSe_2$ and b) orthorhombic unit cell of a $MoSe_2$ supercell, consisting of only 7 OUC, for visibility. The high-symmetry points and the path connecting them are highlighted. c) Multiple supercell BZ covering the reciprocal space, compared to a hexagonal BZ, further illustrating their relationship in the unfolding process. The supercell BZ, and thus all the features of the band structure in that representation are mapped onto the hexagonal one multiple times, resulting in state replicas, with their spectral weight governed by Eq. 2 in the main text. Furthermore, an optical transition in the supercell, with endpoints illustrated by a red line, need not be vertical in the hexagonal BZ.

S2. FOLDED BAND STRUCTURES OF THE NANOWRINKLES

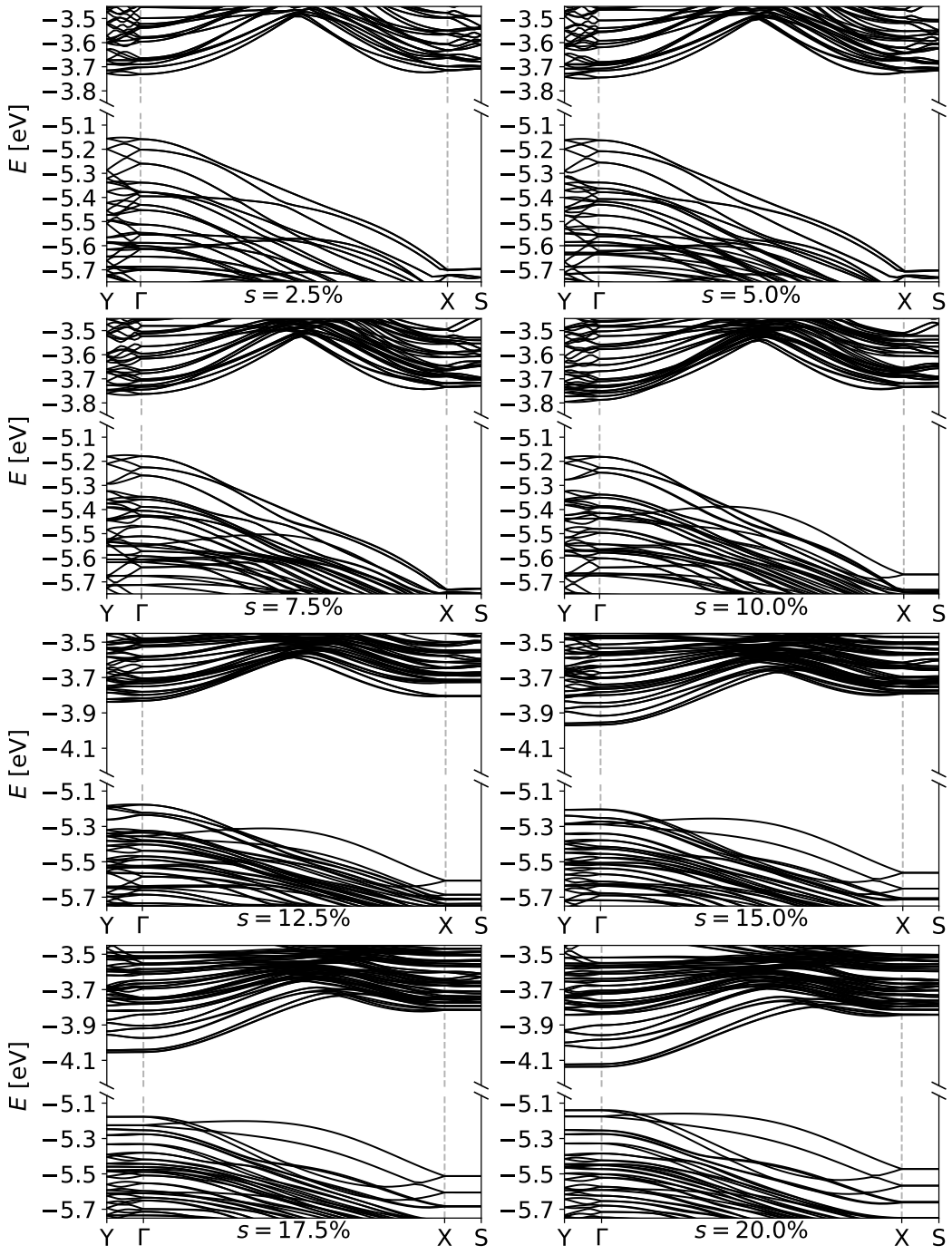

FIG. S3. Band structure of the $MoSe_2$ nanowrinkles considered in this work with increasing values of strain s.

S3. UNFOLDED BAND STRUCTURES OF THE NANOWRINKLES

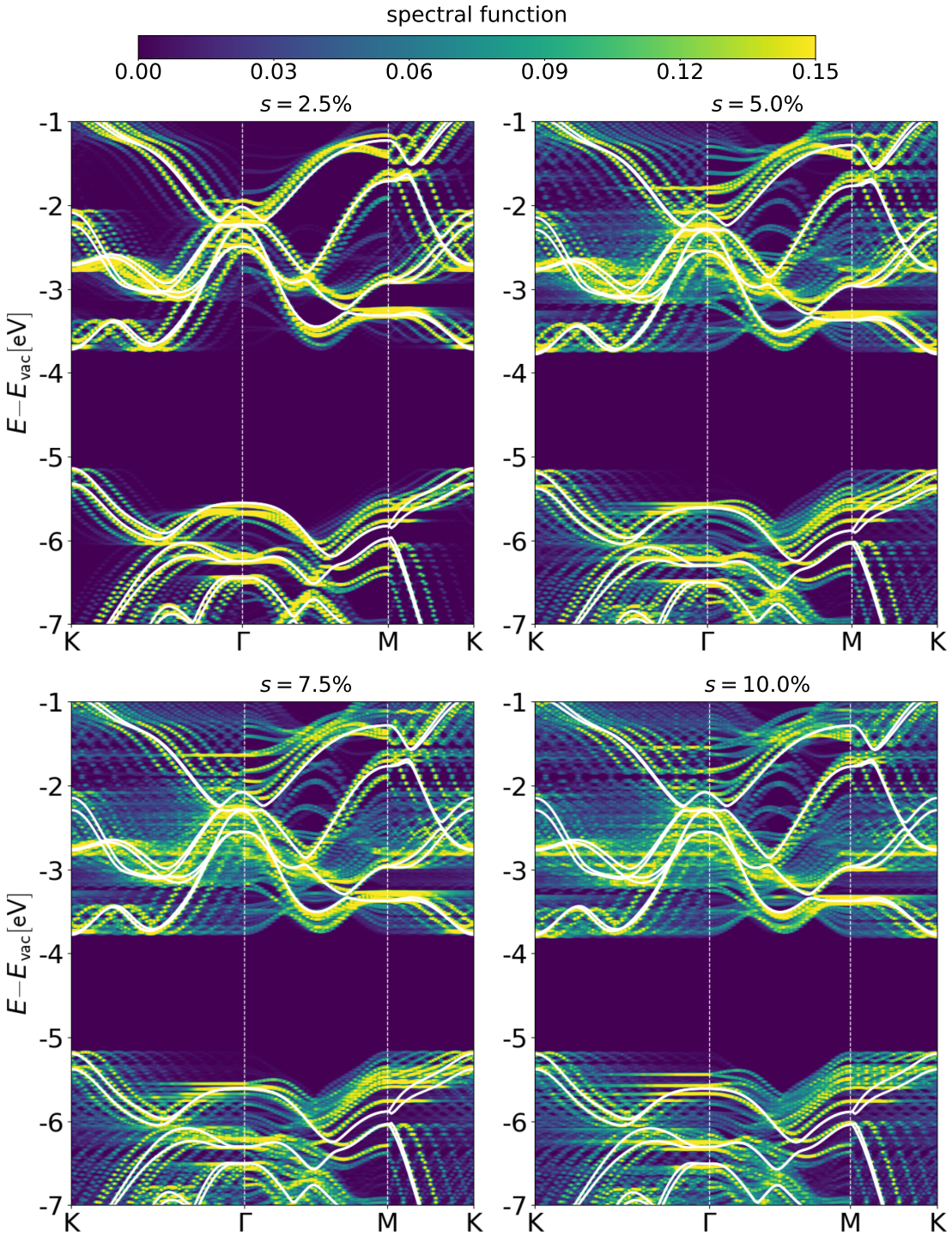

FIG. S4. Band structure of the $MoSe_2$ nanowrinkles with $s = 2.5\%$, $s = 5.0\%$, $s = 7.5\%$, and $s = 10.0\%$ in the hexagonal representation. White lines indicate the band structure of the flat, unstrained $MoSe_2$ monolayer.

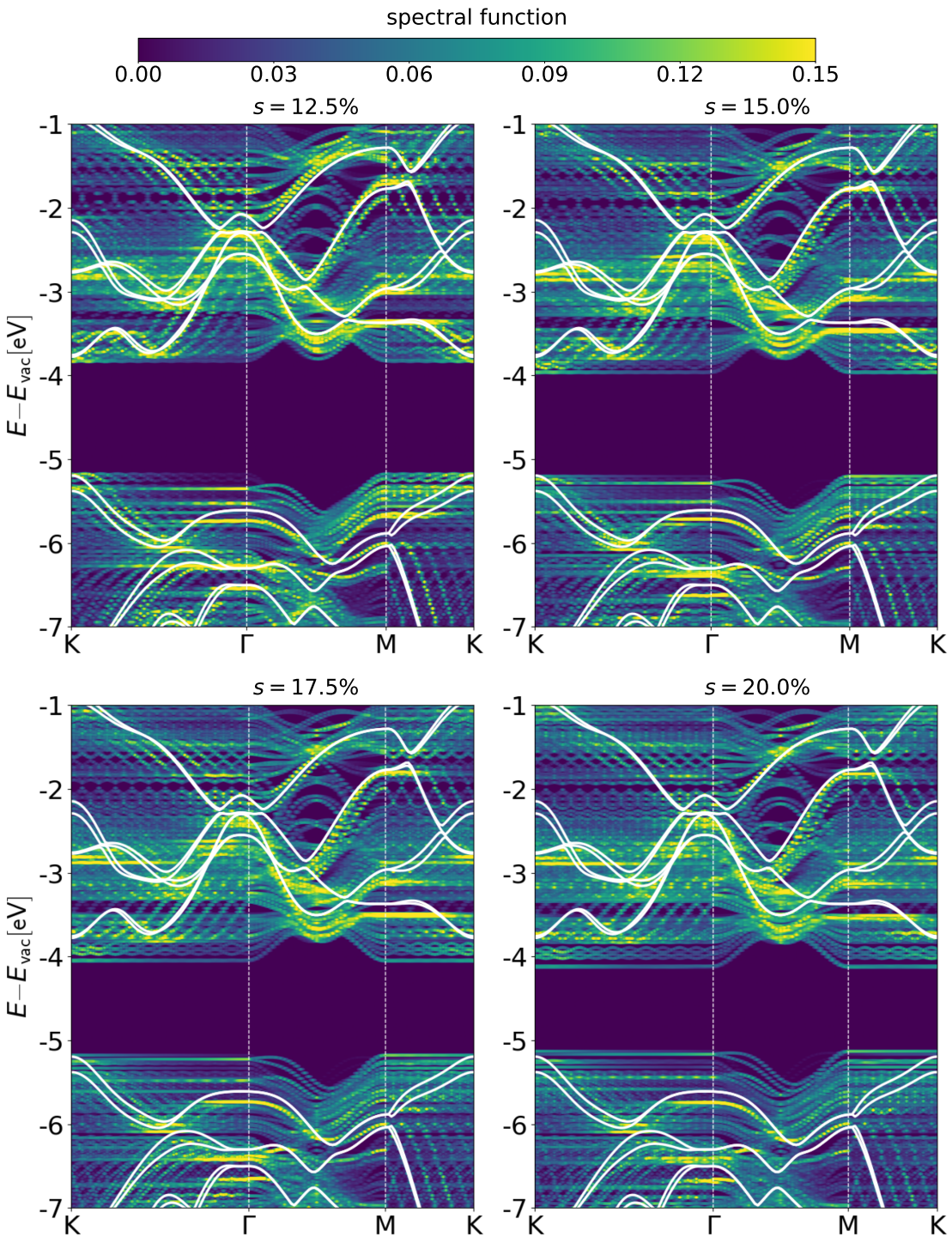

FIG. S5. Band structure of the $MoSe_2$ nanowrinkles with $s = 12.5\%$, $s = 15.0\%$, $s = 17.5\%$, and $s = 20.0\%$ in the hexagonal representation. White lines indicate the band structure of the flat, unstrained $MoSe_2$ monolayer.

S4. FLAT MONOLAYERS UNDER STRAIN

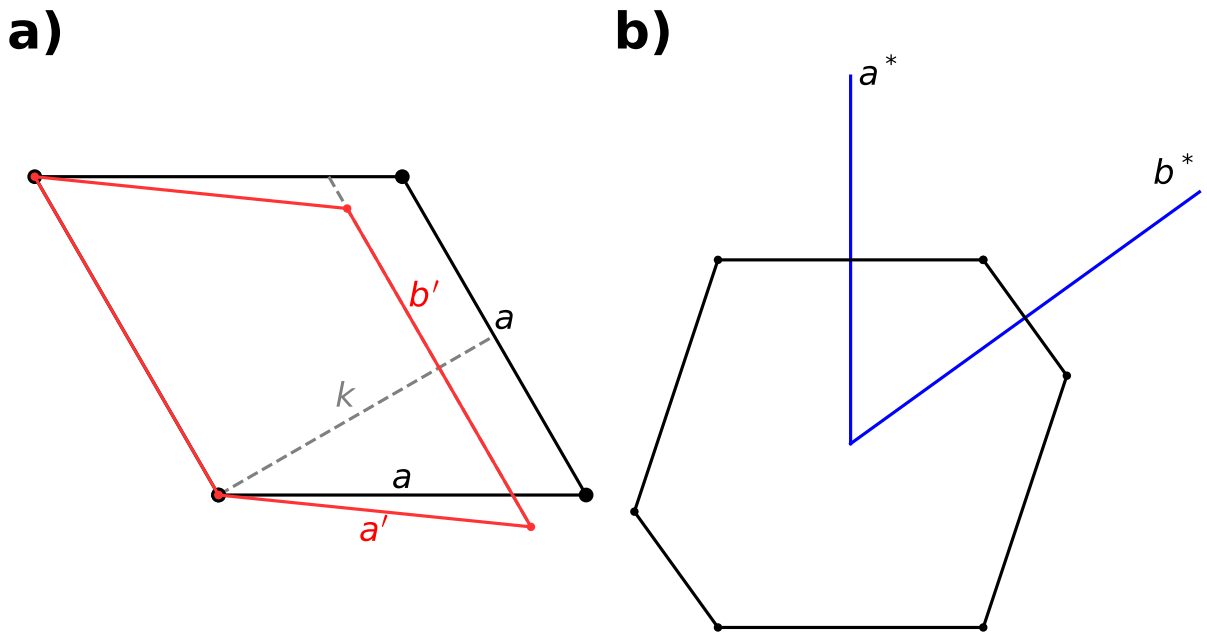

FIG. S6. a) Sketch of the primitive unit cell of $MoSe_2$ (black) of the corresponding flat monolayer under 20% strain (red). The vector **k** along which strain is applied is shown by a gray dashed line. b) First BZ of the strained unit cell with the two reciprocal lattice vectors marked in blue.

The unit cell of the flat $MoSe_2$ monolayer under strain is shown in red in Figure S6a) and compared against the pristine representation (black). The uniaxial strain s is applied along the vector **k**, which is perpendicular to lattice vector **b**. The resulting unit cell is not only compressed but also its angles are modified. This deformation is consequently reflected in the first BZ (see Figure S6b). In Figure S7, the band structures of the flat $MoSe_2$ monolayer under increasing values of strain are shown.

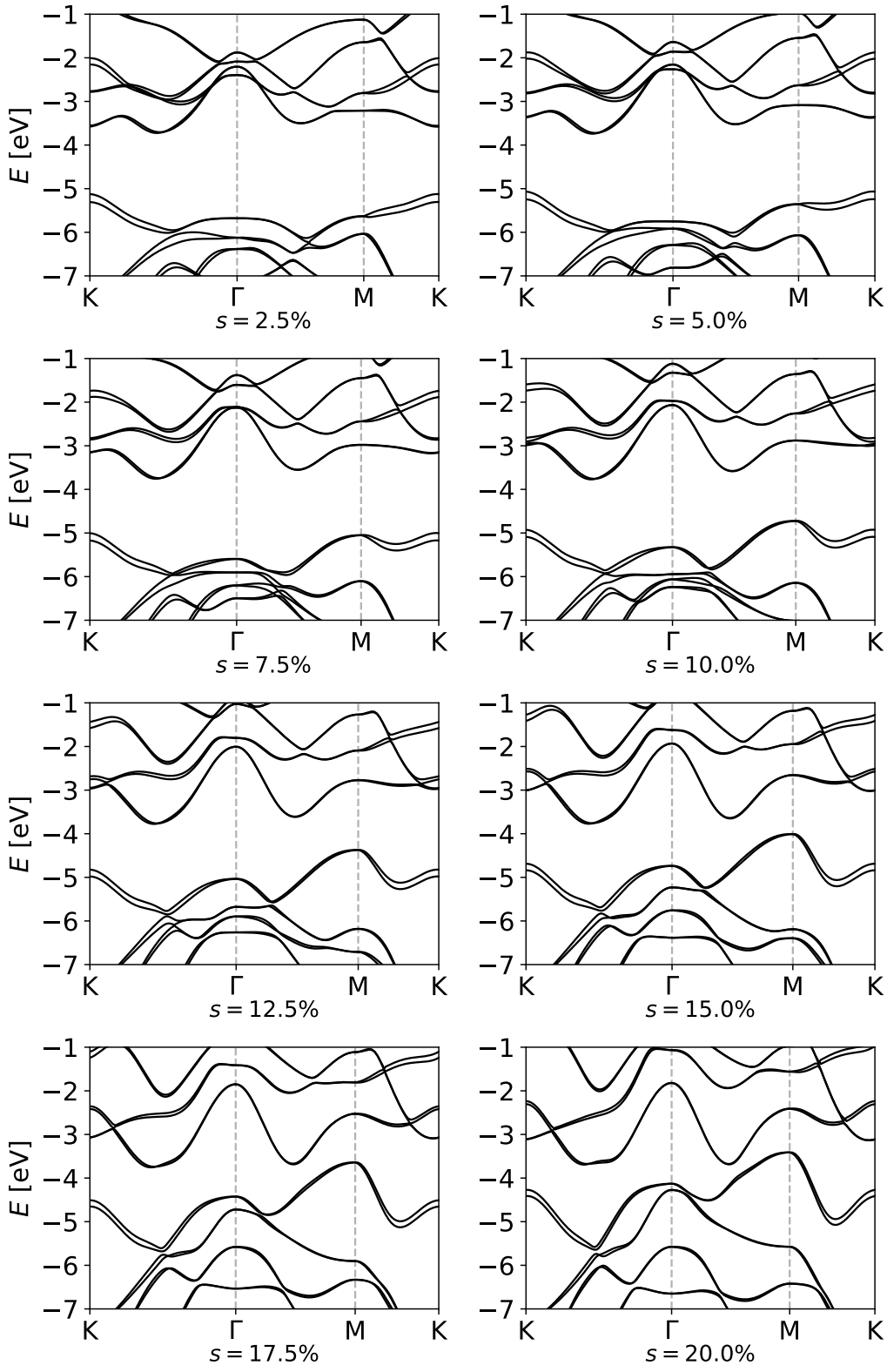

FIG. S7. Band structures of the flat, uniaxially strained $MoSe_2$ monolayers for all the examined values of s.

S5. EFFECTIVE MASS AND WAVE-FUNCTION DISTRIBUTION

In Figure S8, we display the effective masses computed for the three lowest unoccupied bands in the considered nanowrinkles at varying strain s.

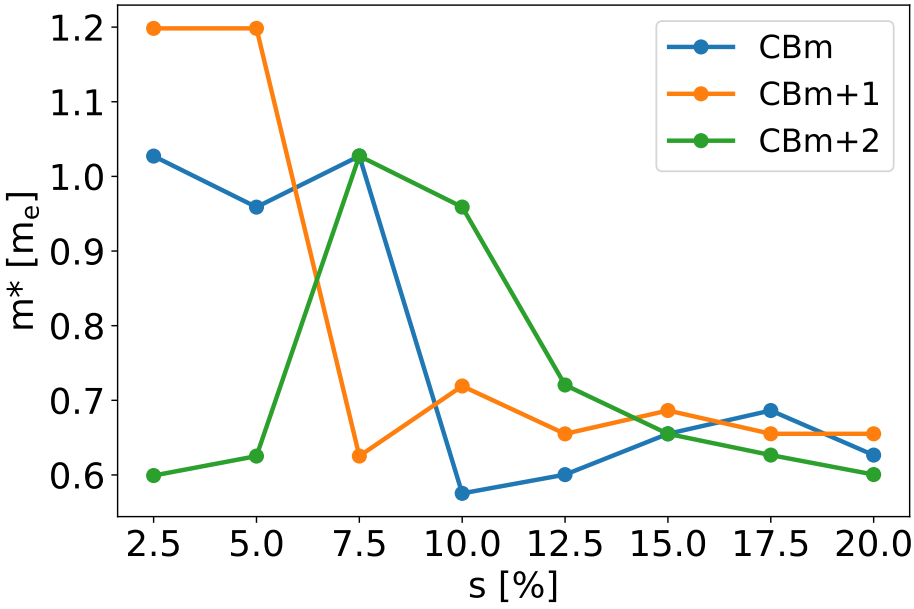

FIG. S8. Effective mass m^* of the lowest, second lowest and third lowest unoccupied states at Γ.

In Figures S9, S10, S11, and S12, we visualize the wave-function distribution (WFD) of the top valance state and of the three lowest unoccupied at Γ, respectively.

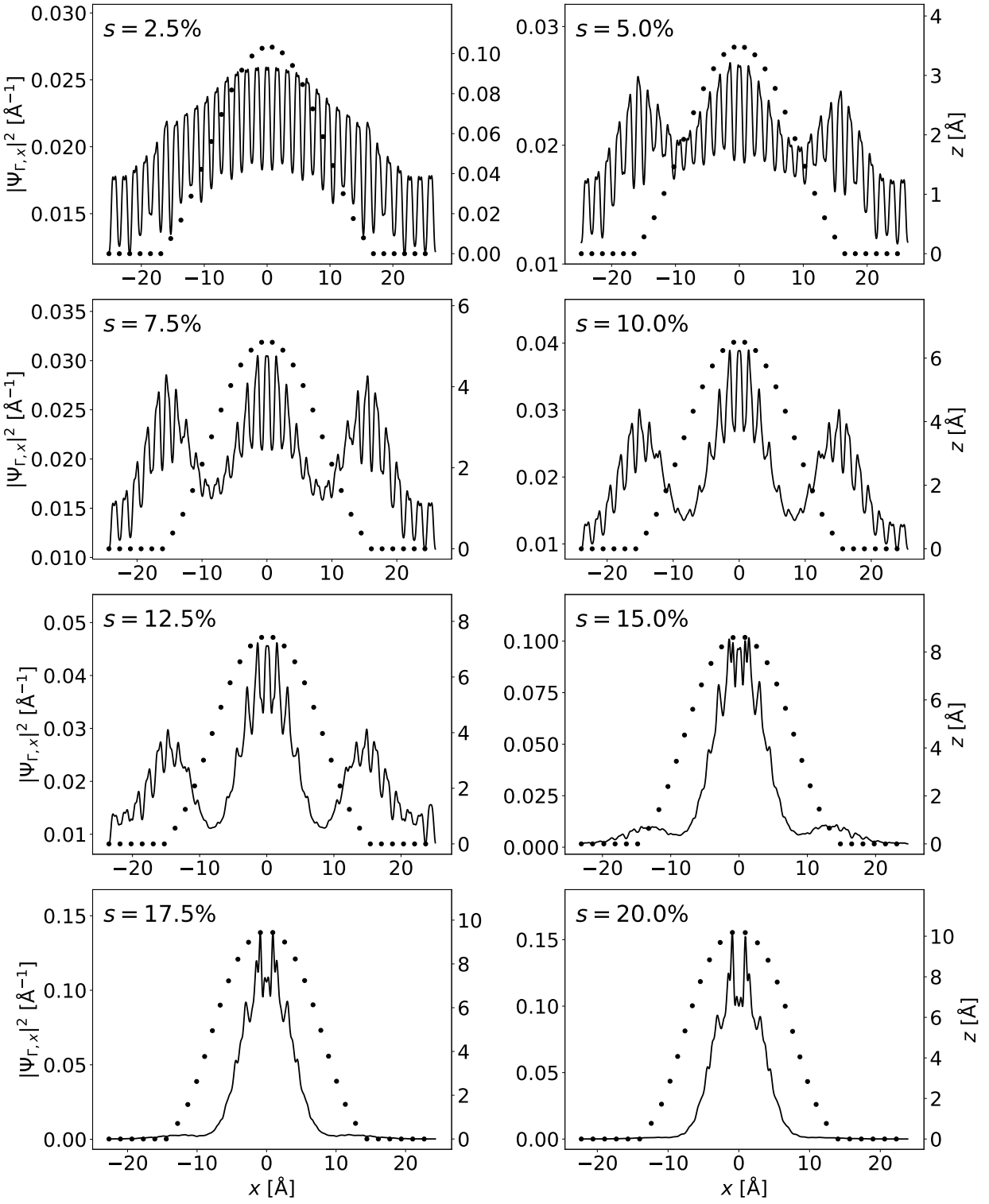

FIG. S9. Wave function distribution of electrons averaged in the (y, z)-plane throughout the nanowrinkle, at the highest-occupied state at the Γ point, for all examined values of s.

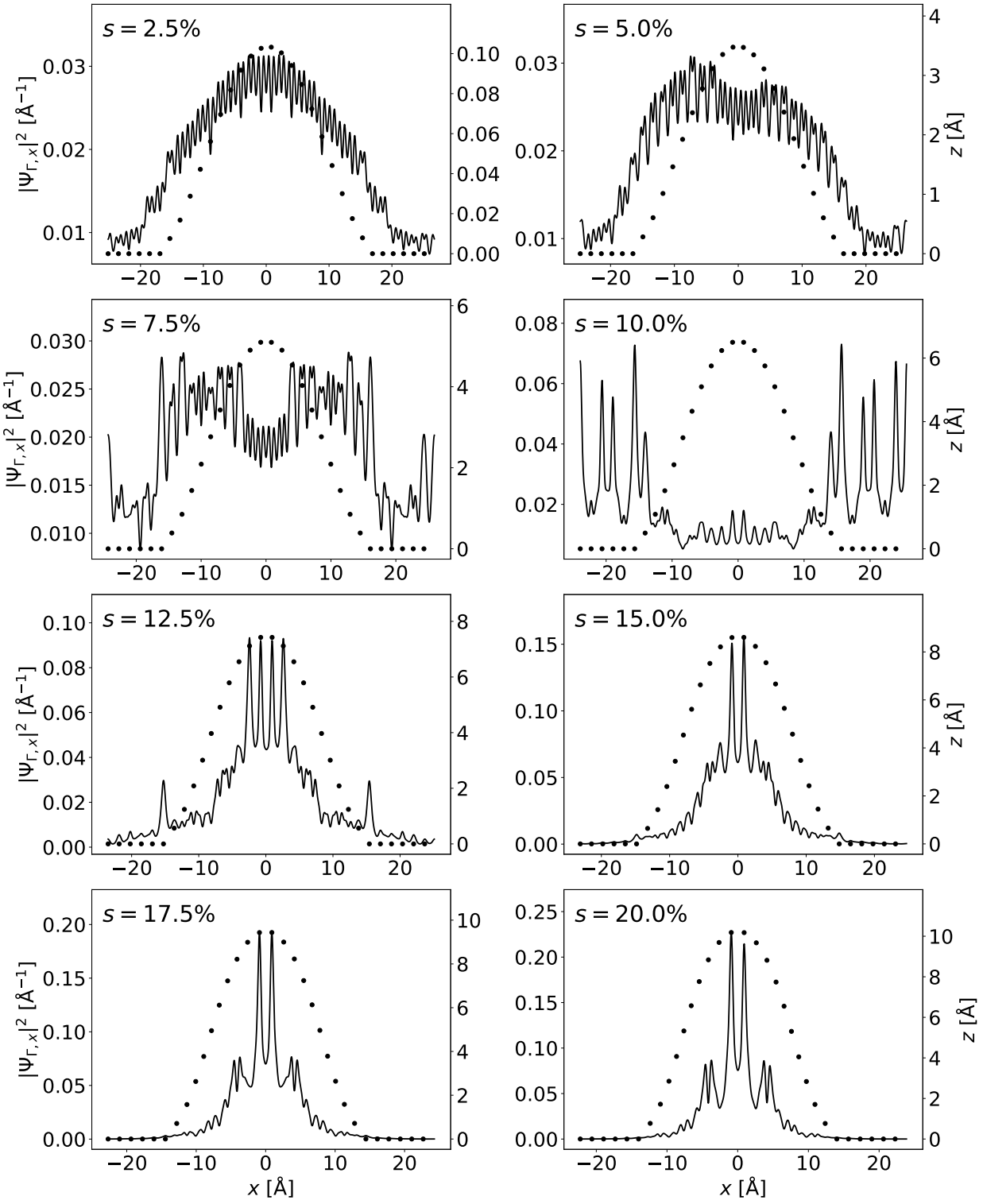

FIG. S10. Wave function distribution of electrons averaged in the (y, z)-plane throughout the nanowrinkle, at the lowest-unoccupied state at the Γ point, for all examined values of s.

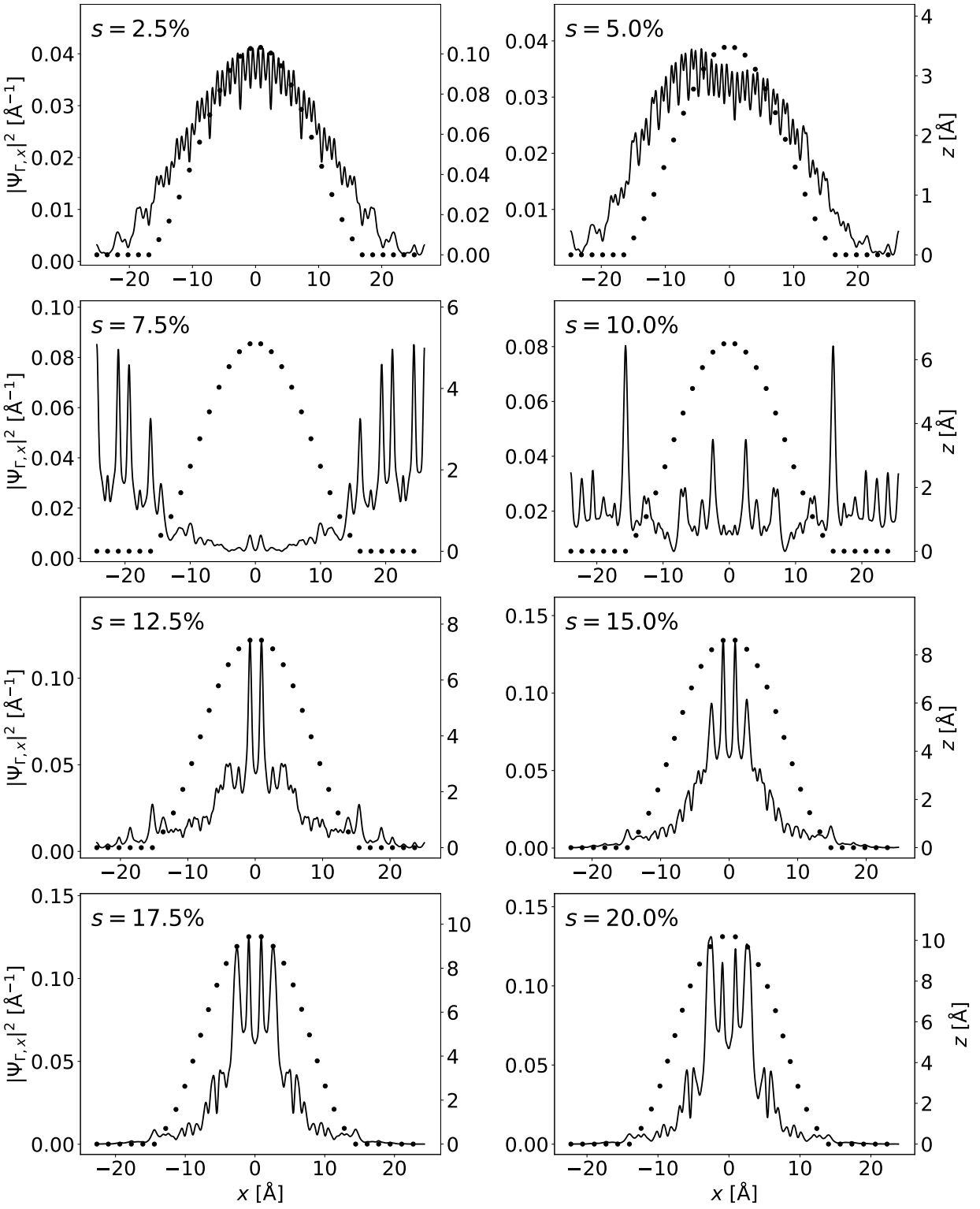

FIG. S11. Wave function distribution of electrons averaged in the (y, z)-plane throughout the nanowrinkle, at the second lowest-unoccupied state at the Γ point, for all examined values of s.

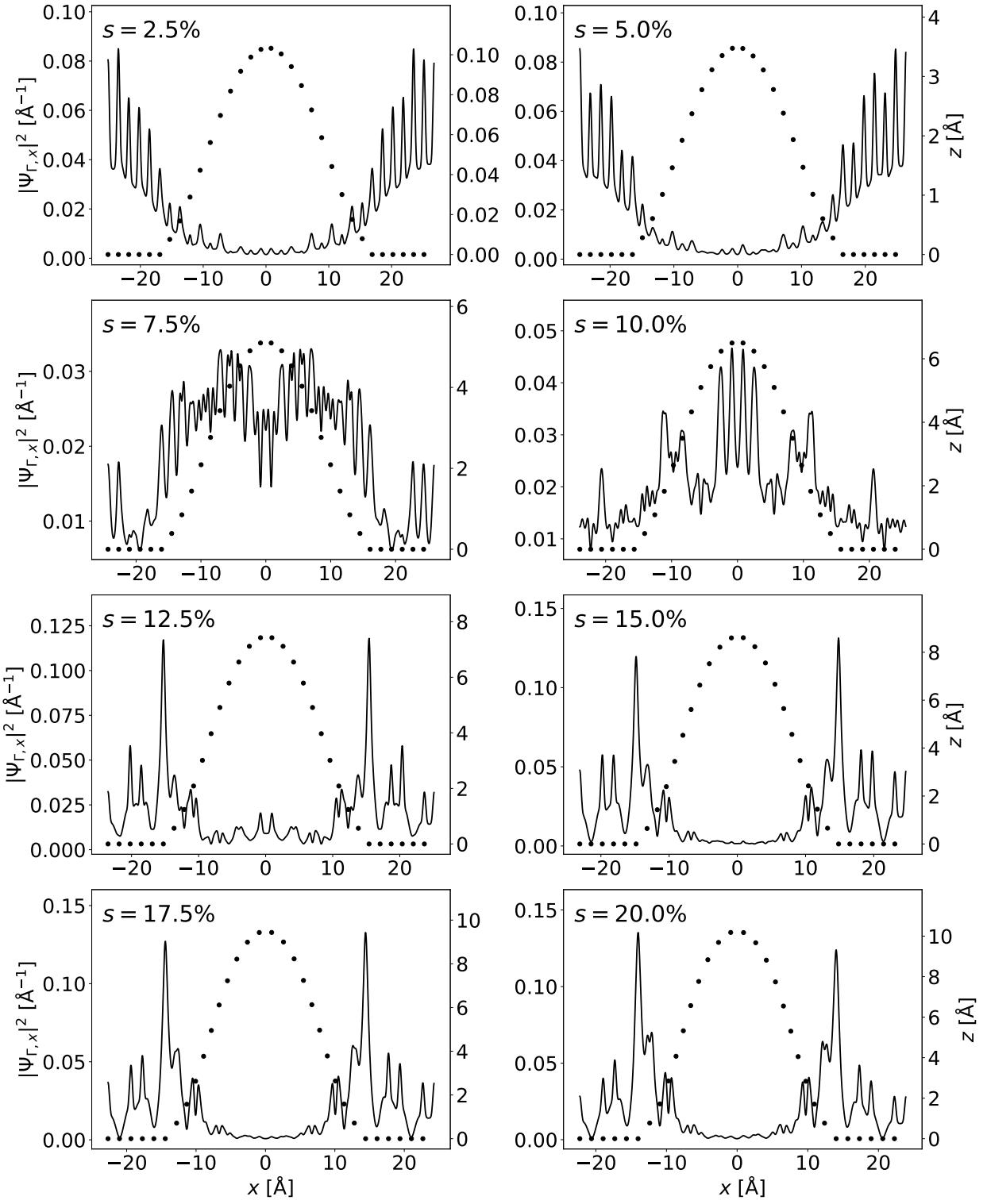

FIG. S12. Wave function distribution of electrons averaged in the (y, z)-plane throughout the nanowrinkle, at the third lowest-unoccupied state at the Γ point, for all examined values of s.

We aim to correlate effective mass and WFD in the considered $MoSe_2$ nanowrinkles. To do so, it is instructive to differentiate among localized states, where most of the probability density is localized either at the peak or in the periphery of the nanowrinkle (see Fig. S9, $s = 20\%$), delocalized states, where the wave function is almost equally distributed over the entire system (Fig. 10, $s = 2.5\%$), and intermediate states, which we call hereafter "semi-localized" and which are exemplified in Figs. S11 and S12 by the plots for $s = 10\%$.

To perform this analysis, we first split the supercell into an inner and an outer section. The outer section contains the leftmost and rightmost segments of the unit cell, each of length $A \cdot (2.5 + 2(1 - s))$, where $a \approx 3.30$ Å is the primitive lattice constant. The rest of the supercell makes up the inner section. Next, we integrate the WFD in both sections separately to obtain I_{in} and I_{out}, with $I_{\text{in}} + I_{\text{out}} = 1$. We define σ as the normalized standard deviation (SD) of the WFD in the inner section if $I_{\text{in}} > 0.6$, the SD in the outer section if $I_{\text{out}} > 0.6$ and as the SD throughout the whole wrinkle otherwise. The SD is used as a measure of the sharpness of the WFD curve, which is more pronounced in strongly localized states. We introduce the parameter M, similar to Moran's I [2], defined as:

$$M = \frac{N}{W} \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij}(f_i - \bar{f})(f_j - \bar{f})}{\sum_{i=1}^{N}(f_i - \bar{f})^2}, \tag{S1}$$

where $N = 1000$ is the number of discrete units in which the WFD can be discretized, $f = |\Psi_{\Gamma,x}|^2$, and $\bar{f}$ is the mean value of f across the supercell; $w_{ij} = \max(d_0 - d(i,j), 0)$ is a matrix assigning weights to pairs of spatial indices based on their distance $d(i,j)$, which takes periodic boundary conditions into account so that $d(i,j) = \min(|i-j|, N - |i-j|)$; $d_0 = 31$ is the rounded average distance between two neighboring Mo atoms, expressed through the number of elementary units of length used for the discretization of the space; finally, $W = \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij}$ is the sum of all elements in the weight matrix. With the aid of σ and M, we can define a localization parameter L for any state i:

$$L_i = |M_i - \sigma_i|. \tag{S2}$$

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[1] A. Kokalj, Xcrysden—a new program for displaying crystalline structures and electron densities, J. Mol. Graphics Modell. **17**, 176 (1999).

[2] P. A. Moran, Notes on continuous stochastic phenomena, Biometrika **37**, 17 (1950).