Supporting information for: Tuning of the surface exposing and photocatalytic activity for AgX(X=Cl and Br): a theoretical study

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Table 1: The list of Monkhorst-Pack k-point grids used for final energy calculations of different supercell models of (100), (110), and (111) surfaces for AgCl.

Slab model	k-point set
S(100)-1 × 2	$12 \times 8 \times 1$
S(100)-1 × 3	$12 \times 6 \times 1$
S(100)-1 × 4	$12 \times 4 \times 1$
S(110)-1 × 2	$10 \times 6 \times 1$
S(110)-1 × 3	$10 \times 4 \times 1$
S(110)-1 × 4	$10 \times 2 \times 1$
S(111)-1 × 2	$12 \times 8 \times 1$
S(111)-1 × 3	$12 \times 6 \times 1$
S(111)-1 × 4	$12 \times 4 \times 1$

Table 2: The list of Monkhorst-Pack k-point grids used for final energy calculations of different supercell models of (100), (110), and (111) surfaces for AgBr.

Slab model	k-point set
S(100)-1 × 1	$10 \times 10 \times 1$
S(100)-1 × 2	$10 \times 6 \times 1$
S(110)-1 × 1	$10 \times 10 \times 1$
S(110)-1 × 2	$10 \times 6 \times 1$
S(111)-1 × 1	$10 \times 10 \times 1$
S(111)-1 × 2	$10 \times 6 \times 1$

Table 3: Calculated surface energy using 18, 10 and 8 layers of slabs for (100) and (110) surfaces; 24, 16 and 14 layers for (111) surfaces for AgCl.

Layers	(100)surface(J/m^2)	(110)surface(J/m^2)	Layers	(111)surface(J/m^2)
8	0.312	0.513	14	1.042
10	0.308	0.511	16	1.046
18	0.300	0.500	24	1.025

Table 4: Calculated surface energy of pure surfaces using different supercells for AgCl

Supercell	(100)surface(J/m^2)	(110)surface(J/m^2)	(111)surface(J/m^2)
(1×1)	0.312	0.513	1.042
(1×2)	0.312	0.513	1.042
(1×3)	0.309	0.513	1.042
(1×4)	0.312	0.512	1.041