

## **Identification of Preferentially Exposed Crystal Facets by X-ray Diffraction**

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Table S1. Selected examples of crystalline materials with preferentially exposed facets and their applications

Material	Preferentially exposed facet(s)	Application	Ref.
Ag <sub>3</sub> PO <sub>4</sub> rhombic dodecahedron	{110}	Photocatalytic degradation of rhodamine B (RhB) and methyl orange (MO)	<sup>1</sup>
Ag <sub>3</sub> PO <sub>4</sub> cube	{100}		
Bi <sub>2</sub> MoO <sub>6</sub> nanosheets	{001}	Photocatalytic removal of NO	<sup>2</sup>
BiOBr nanosheets	{001}	Photocatalytic synthesis of NH <sub>3</sub> using N <sub>2</sub>	<sup>3</sup>
BiOCl nanosheets	{001} or {010}	Photocatalytic degradation of MO	<sup>4</sup>
BiOCl nanosheets	{001}	Photocatalytic RhB degradation	<sup>5</sup>
BiOIO <sub>3</sub> nanoplates	{010} and {100}	Photocatalytic CO <sub>2</sub> reduction	<sup>6</sup>
BiVO <sub>4</sub> sheet	(040)	Photocatalytic H <sub>2</sub> O oxidation	<sup>7</sup>
BiVO <sub>4</sub> nanoplates	(040)	Photocatalytic H <sub>2</sub> O oxidation	<sup>8</sup>
BiVO <sub>4</sub> photoanode	(001)	Photoelectrochemical H <sub>2</sub> O oxidation	<sup>9</sup>
BiVO <sub>4</sub> nanosheets	{010}	Photocatalytic H <sub>2</sub> O oxidation	<sup>10</sup>
CeO <sub>2</sub> nanocubes	{100}	Oxygen storage	<sup>11</sup>
Co <sub>3</sub> O <sub>4</sub> nanosheets	{112}	Catalytic oxidation of trace C <sub>2</sub> H <sub>4</sub>	<sup>12</sup>
Mesoporous Co <sub>3</sub> O <sub>4</sub>	{110}		
Co <sub>3</sub> O <sub>4</sub> dodecahedra	{111}	Photocatalytic CO <sub>2</sub> reduction	<sup>13</sup>
Co <sub>3</sub> O <sub>4</sub> cube	(001)	Anode material for Li-ion batteries	<sup>14</sup>
Co <sub>3</sub> O <sub>4</sub> polyhedra	(001) and (111)		
Co <sub>3</sub> O <sub>4</sub> octahedra	(111)		
Fe <sub>2</sub> O <sub>3</sub> nanosheets	(110)	Lithium storage and photocatalytic H <sub>2</sub> O oxidation	<sup>15</sup>
Fe <sub>2</sub> PO <sub>5</sub> decahedra	{010} and {110}	Electrocatalytic H <sub>2</sub> O oxidation	<sup>16</sup>
Fe <sub>2</sub> PO <sub>5</sub> octahedra	{110}		
CoP	(211)	Electrocatalytic O <sub>2</sub> reduction in zinc-air batteries	<sup>17</sup>
Ni <sub>3</sub> S <sub>2</sub> nanosheets	{210}	Electrocatalyst for overall H <sub>2</sub> O splitting	<sup>18</sup>
Pt nanocubes	{100}	/	<sup>19</sup>
Pt nanotetrahedra	{111}		
Pt hollow nanocubes	{111}	Catalytic O <sub>2</sub> reduction in fuel cells	<sup>20</sup>
Pt nanoplates	(111)	Electrocatalytic O <sub>2</sub> reduction	<sup>21</sup>
TiO <sub>2</sub> polyhedra	{001}	Photocatalytic decomposition of methylene blue	<sup>22</sup>
TiO <sub>2</sub> nanosheets	(001)	Lithium storage for Li-ion batteries	<sup>23</sup>
TiO <sub>2</sub> (anatase) nanobelts	(101)	Photocatalytic degradation of MO	<sup>24</sup>
TiO <sub>2</sub> (anatase) decahedra	{001}	/	<sup>25</sup>
TiO <sub>2</sub> (anatase) decahedra	{101}	Photocatalytic reduction of fluorogenic molecules	<sup>26</sup>
TiO <sub>2</sub> (anatase) decahedra	{001} or {101}	Photocatalytic conversion of CH <sub>3</sub> OH into H <sub>2</sub>	<sup>27</sup>

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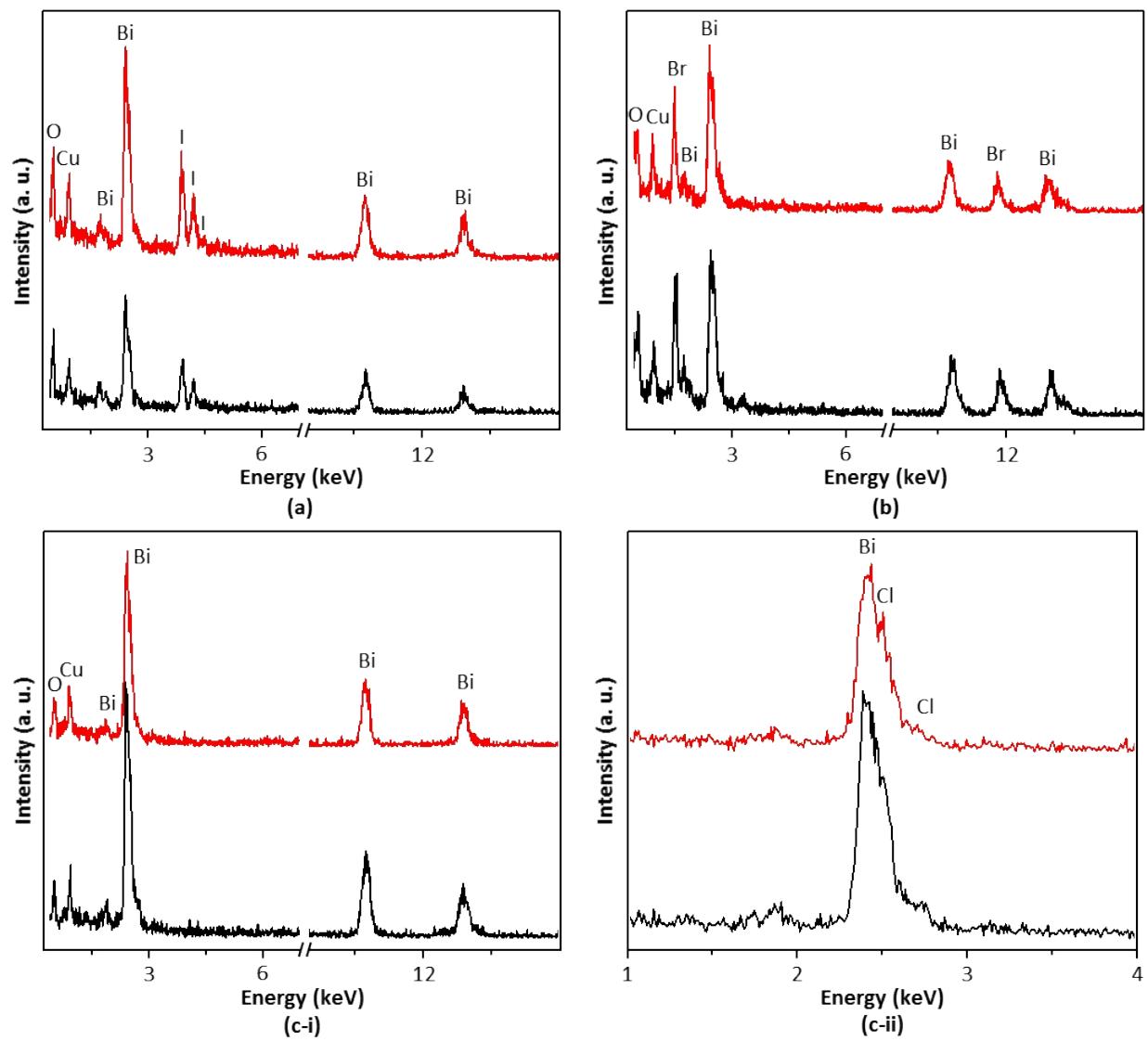


Fig. S1 EDX spectra recorded at two different areas of the synthesized (a) BiOI, (b) BiOBr, and (c) BiOCl samples. The peaks of Cu are attributable to the use of Cu grids.

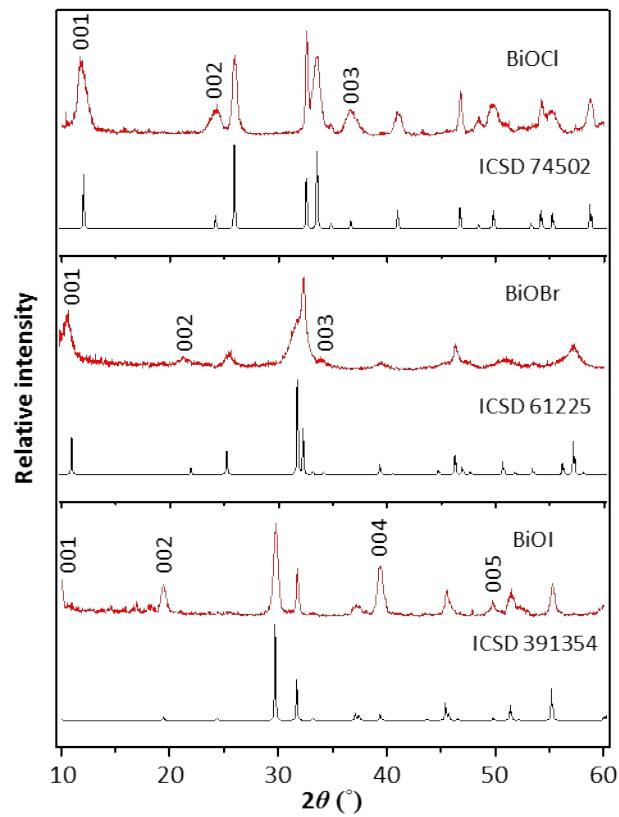


Fig. S2 XRD patterns of the synthesized BiOX samples.

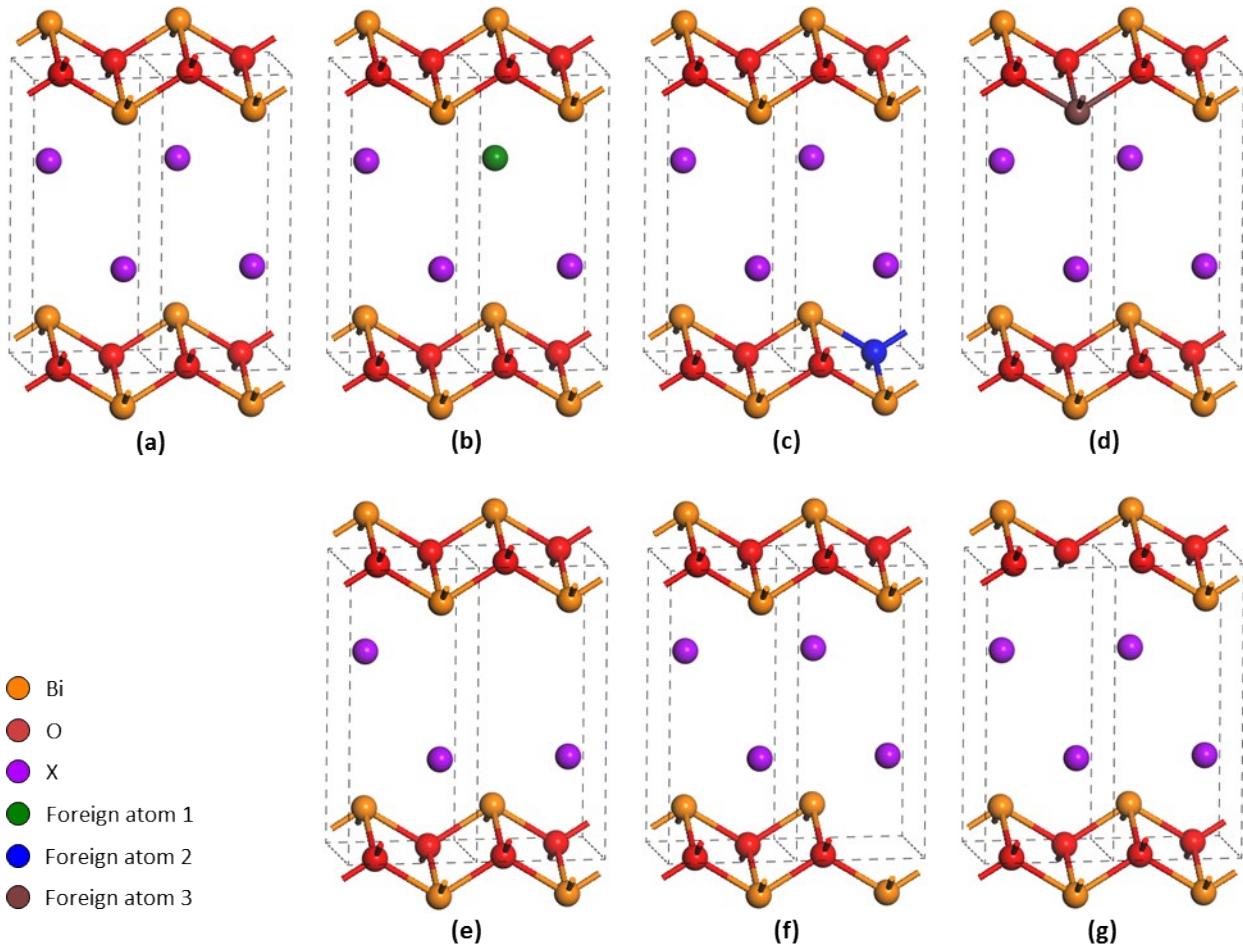


Fig. S3 Crystal structures of (a) BiOX, (b)-(d) BiOX doped with foreign ions, and (e-g) BiOX with vacancies.

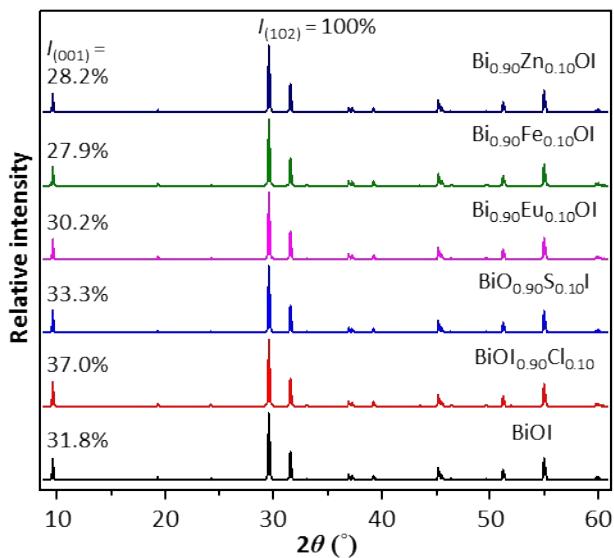


Fig. S4 Simulated XRD patterns of BiOI doped with various elements.

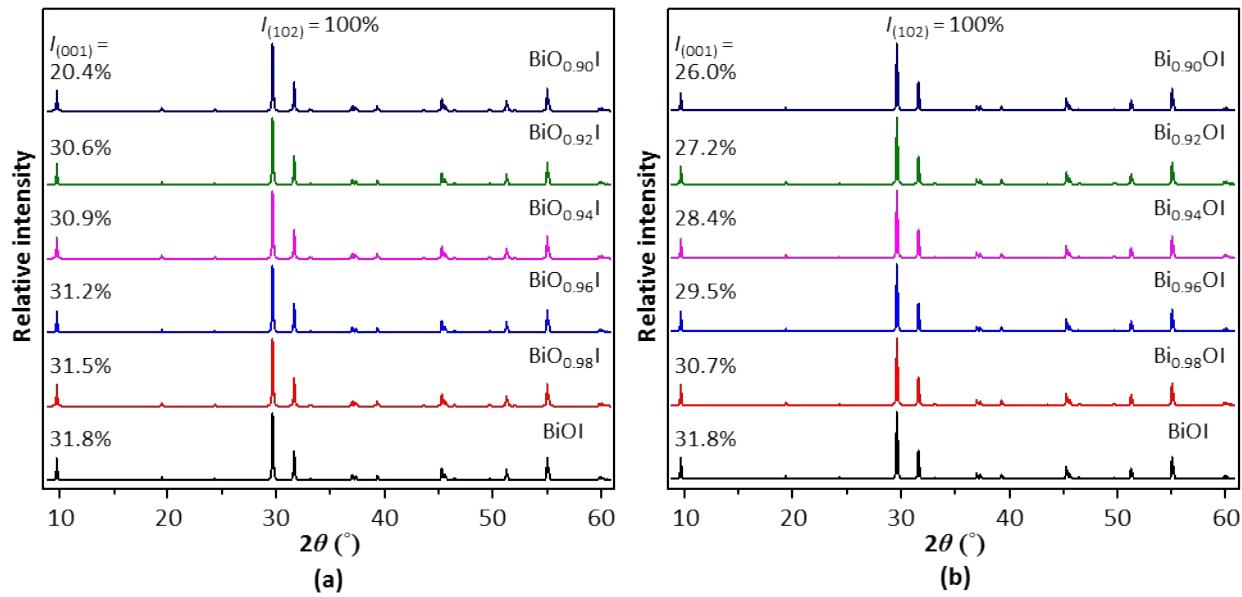


Fig. S5 Simulated XRD patterns of BiOI with various amounts of (a) O and (b) Bi vacancies.

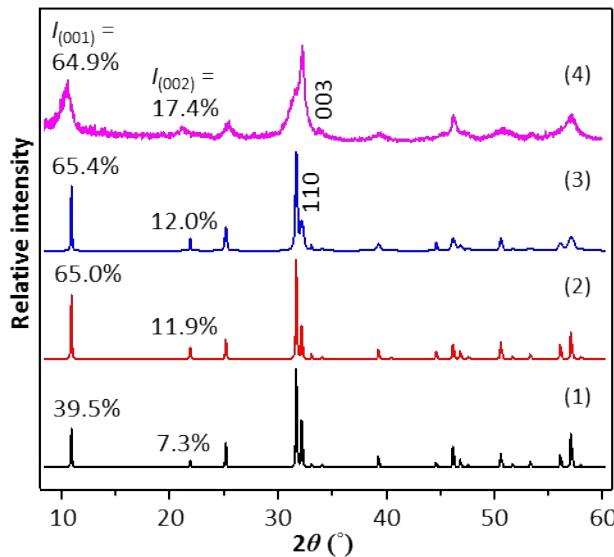


Fig. S6 Simulated (1-3) and experimental (4) XRD patterns of BiOBr. Pattern 1, bulk BiOBr without preferred orientation or anisotropic broadening; pattern 2, preferred orientation in [001] (March/Dollase parameter = 0.828); pattern 3, (110) broadening (anisotropic parameter = 1.5).

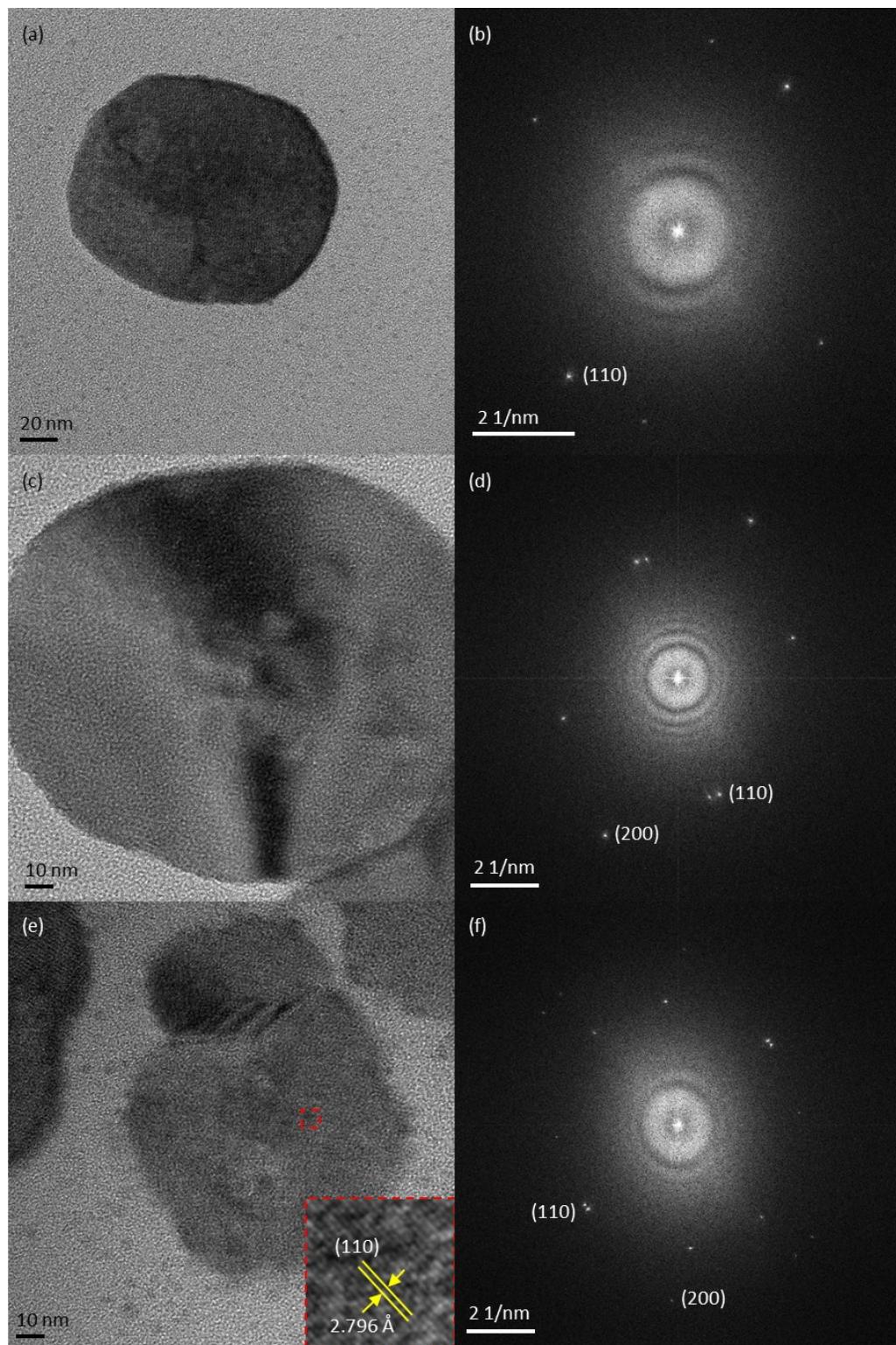


Fig. S7 (a, c, e) TEM images of BiOI nanoplates and (b, d, f) the corresponding fast Fourier transforms (FFTs). The insert of (e) is the magnified image of the red frame-enclosed area.

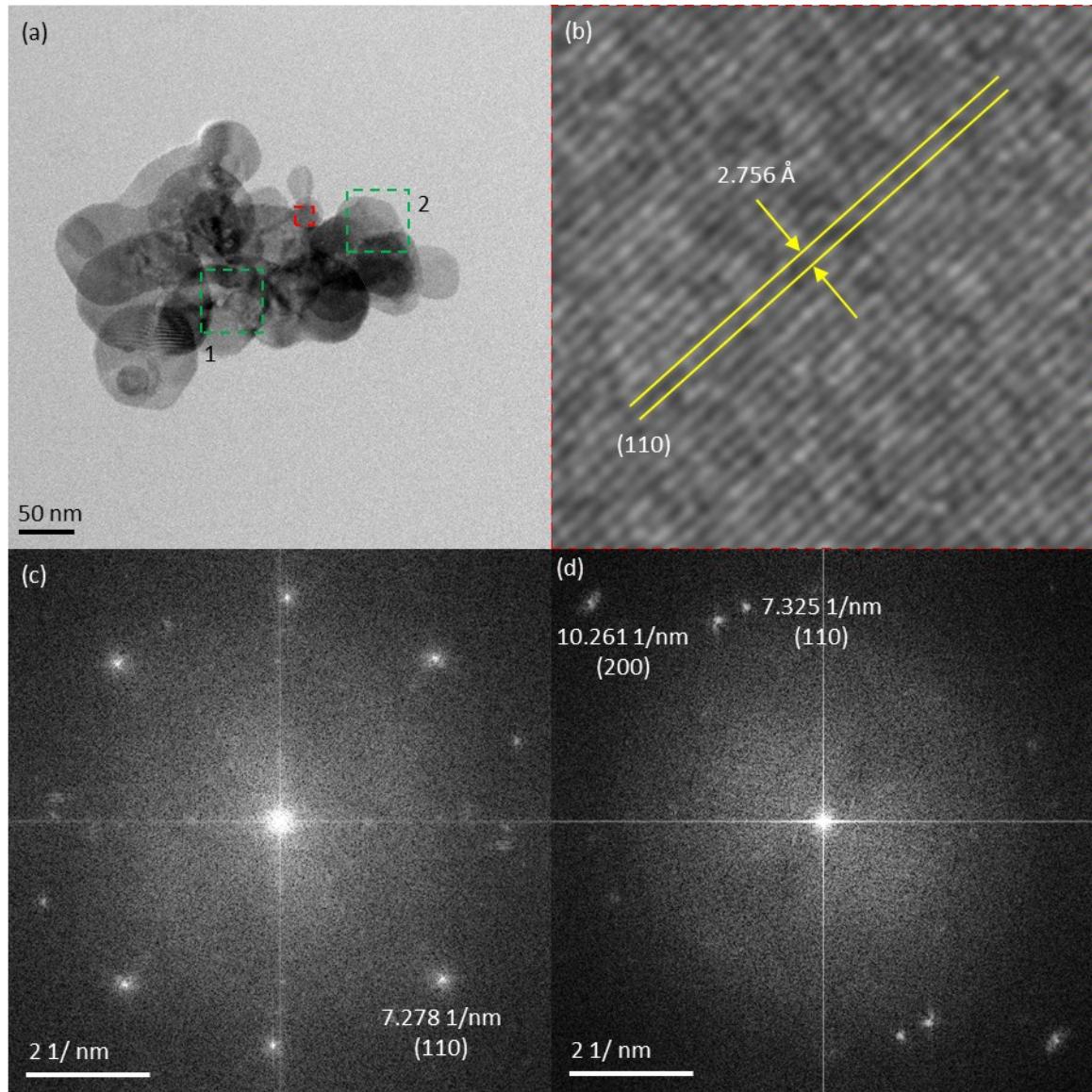


Fig. S8 (a) TEM image of BiOCl, (b) magnified image of the red frame-enclosed area, (c) and (d) FFTs of the green-colored frames 1 and 2, respectively, in (a).