Supporting Information

Atomic bonding and Electronic binding energy of two-dimensional Bi/Li(110) heterojunctions via BOLS-BB model

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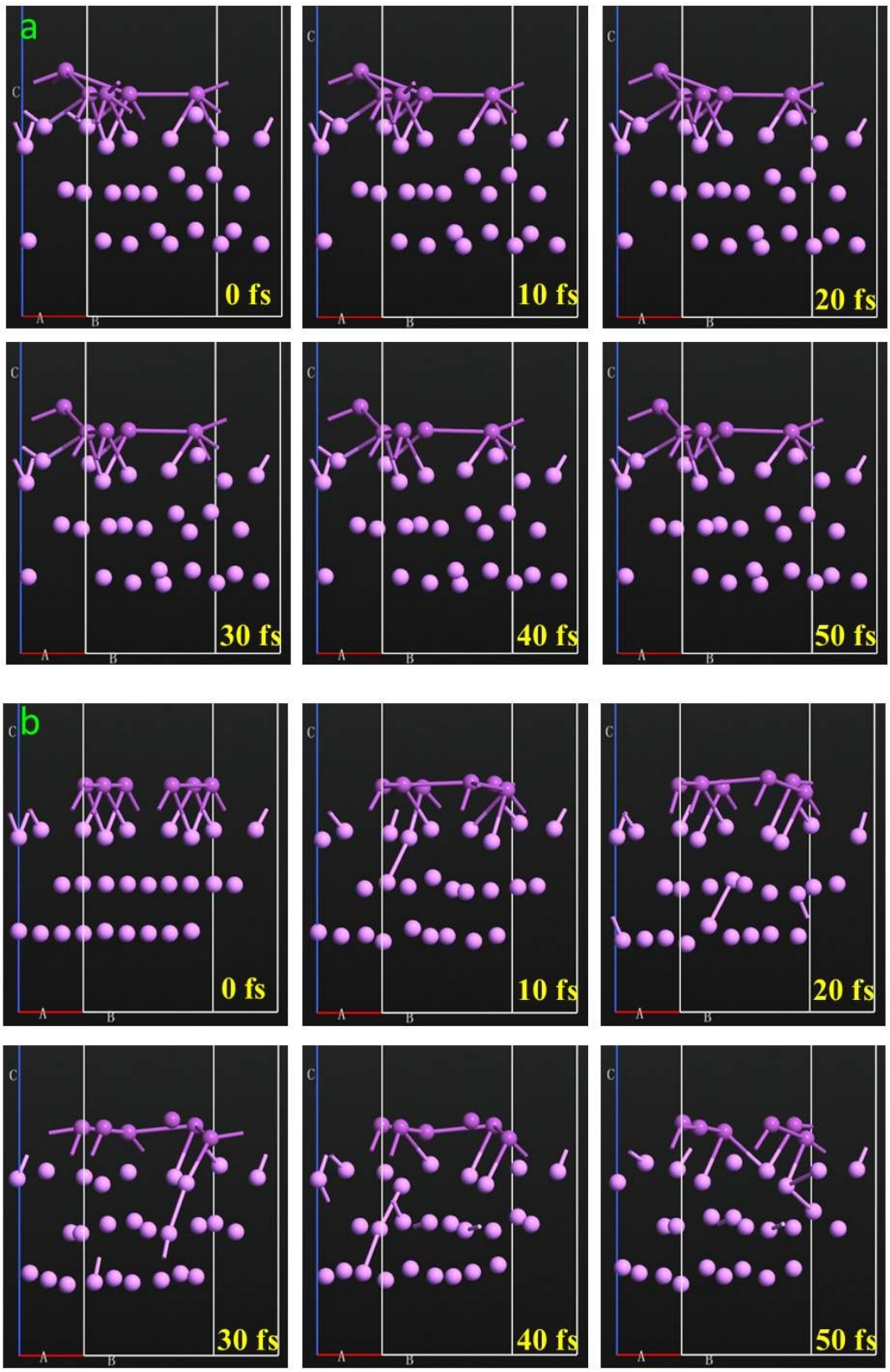
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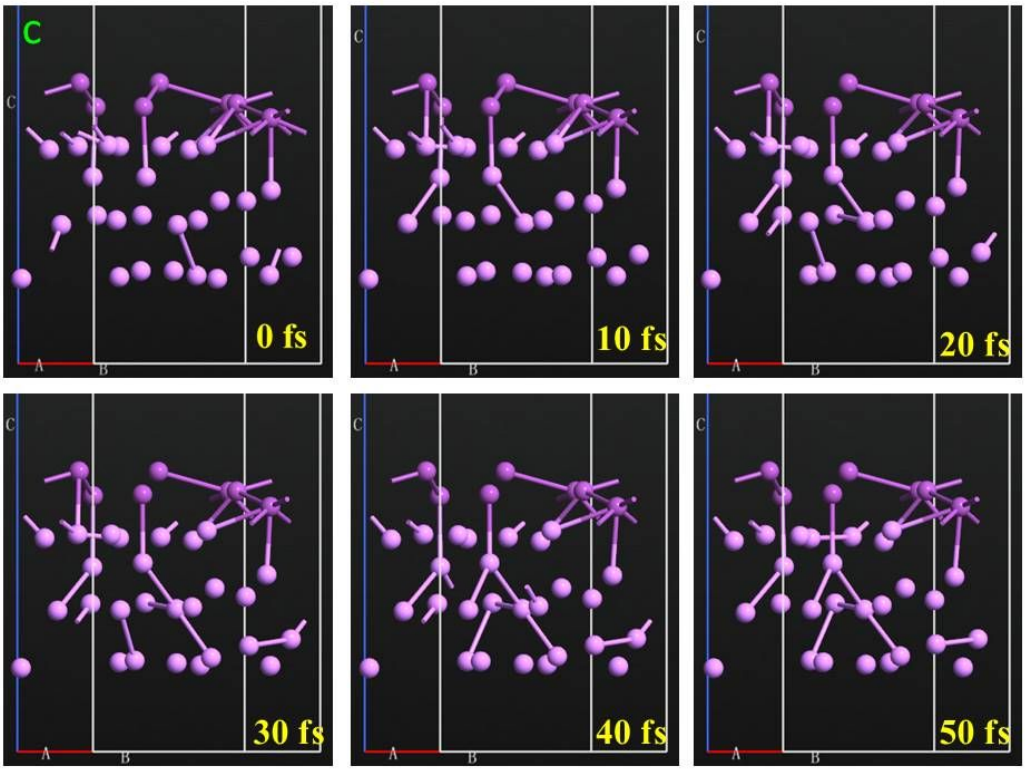
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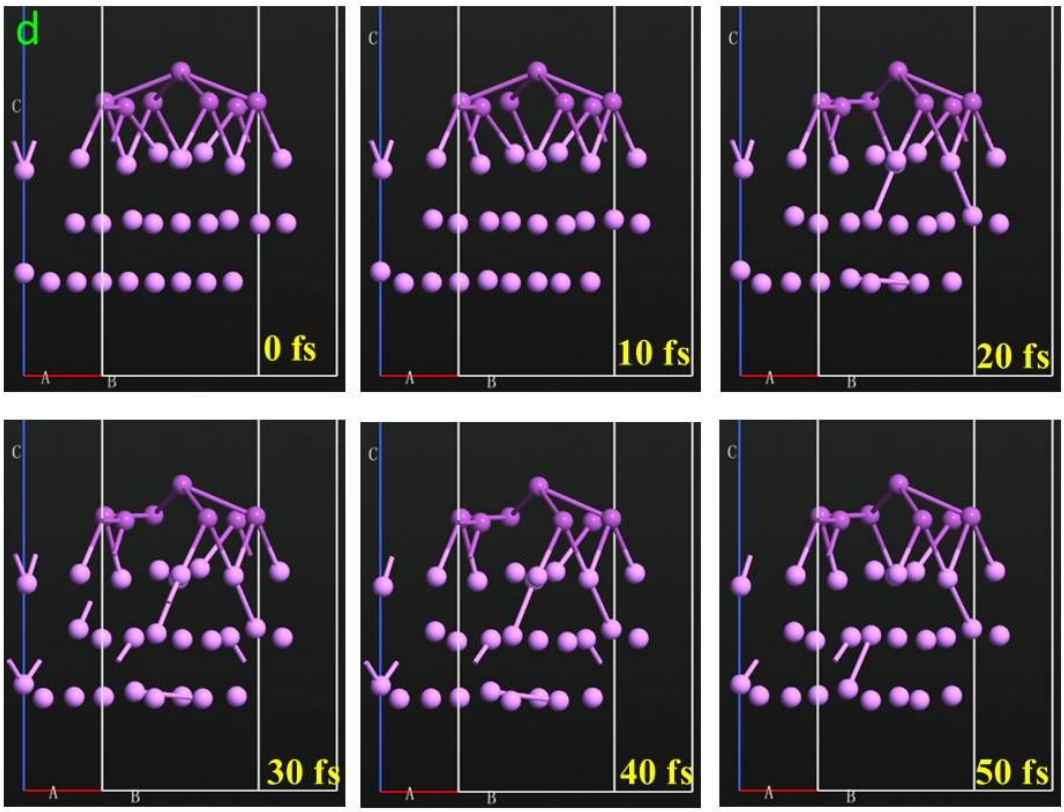
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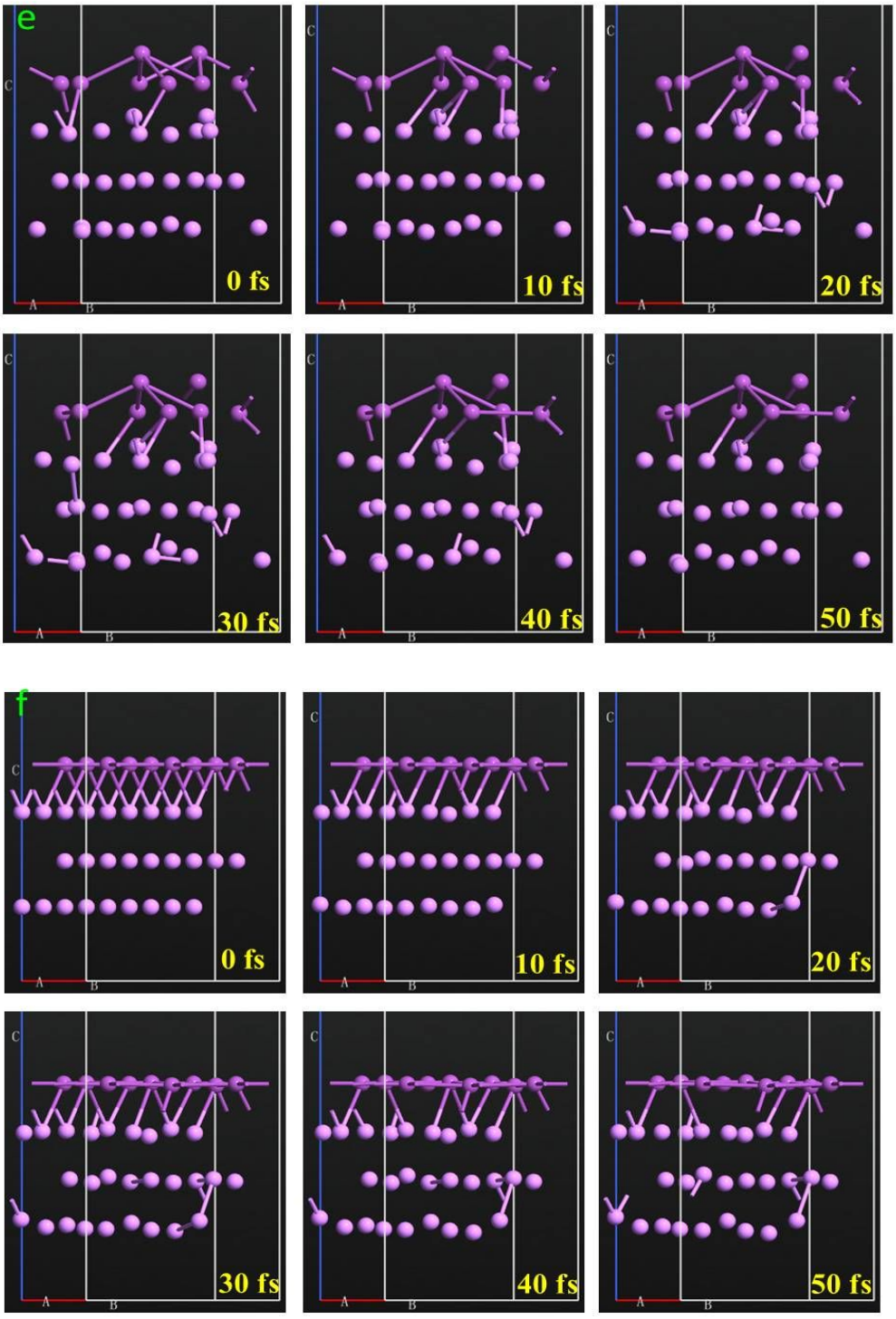

Figure S1. The ab initio molecular dynamics calculations show that the structure of Bi atoms on Li (1 1 0) surfaces, (a) letter shape, (b) hexagon shape, (c) cobweb shape, (d) galaxy shape, (e) crown shape, and (f) field shape. The ab initio molecular dynamics calculations show that the structure is stable. The ab initio molecular dynamics simulations show that there is agglomeration of Bi atoms on the interface.