

## Supplementary Material (SM)

### Catalytic Decomposition of Ammonium Perchlorate at BpyNO

#### Interfaces: A Neural Network Potential Perspective

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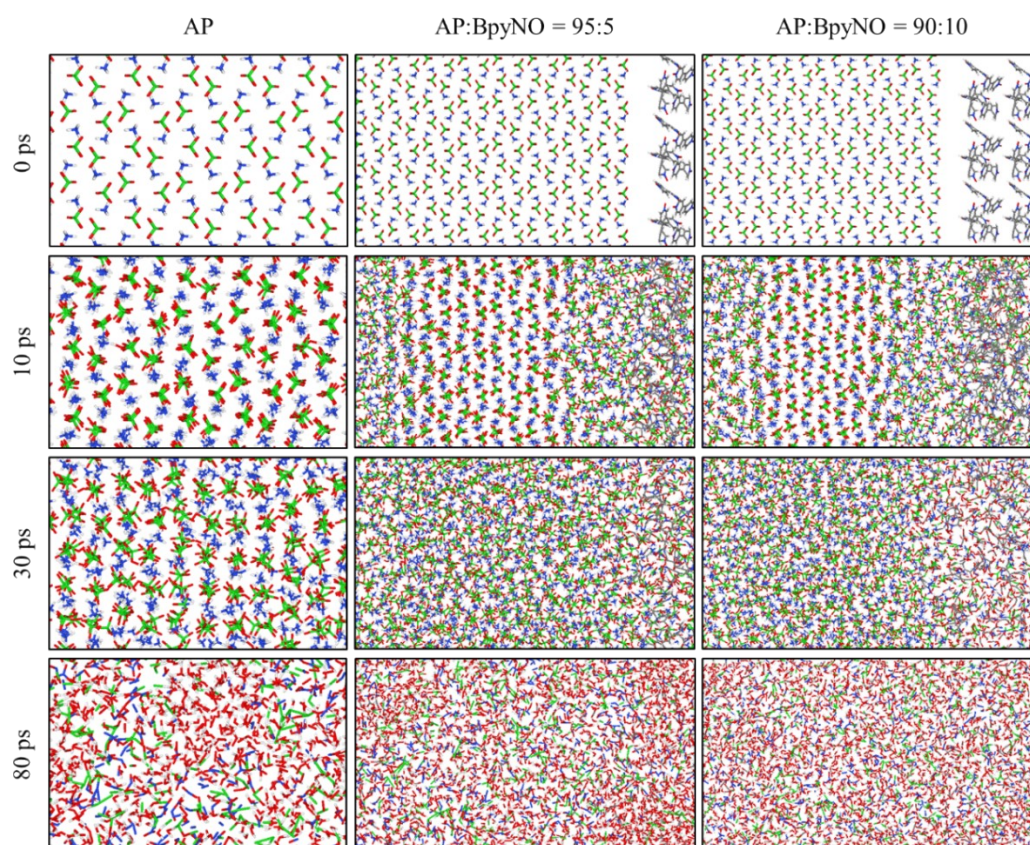
In the supplementary materials, we present:

1. **Figure S1** Morphology of AP and AP/BpyNO composites during heating. The C, H, N, O, and Cl atoms are represented in gray, white, blue, red, and green, respectively.
2. **Figure S2** Decomposition mechanism of AP.
3. **Figure S3** Decomposition mechanism of BpyNO.
4. **Figure S4** Initial decomposition products (left) and major gas-phase products (right) of AP/Bpy (a) and AP/Bph (b).

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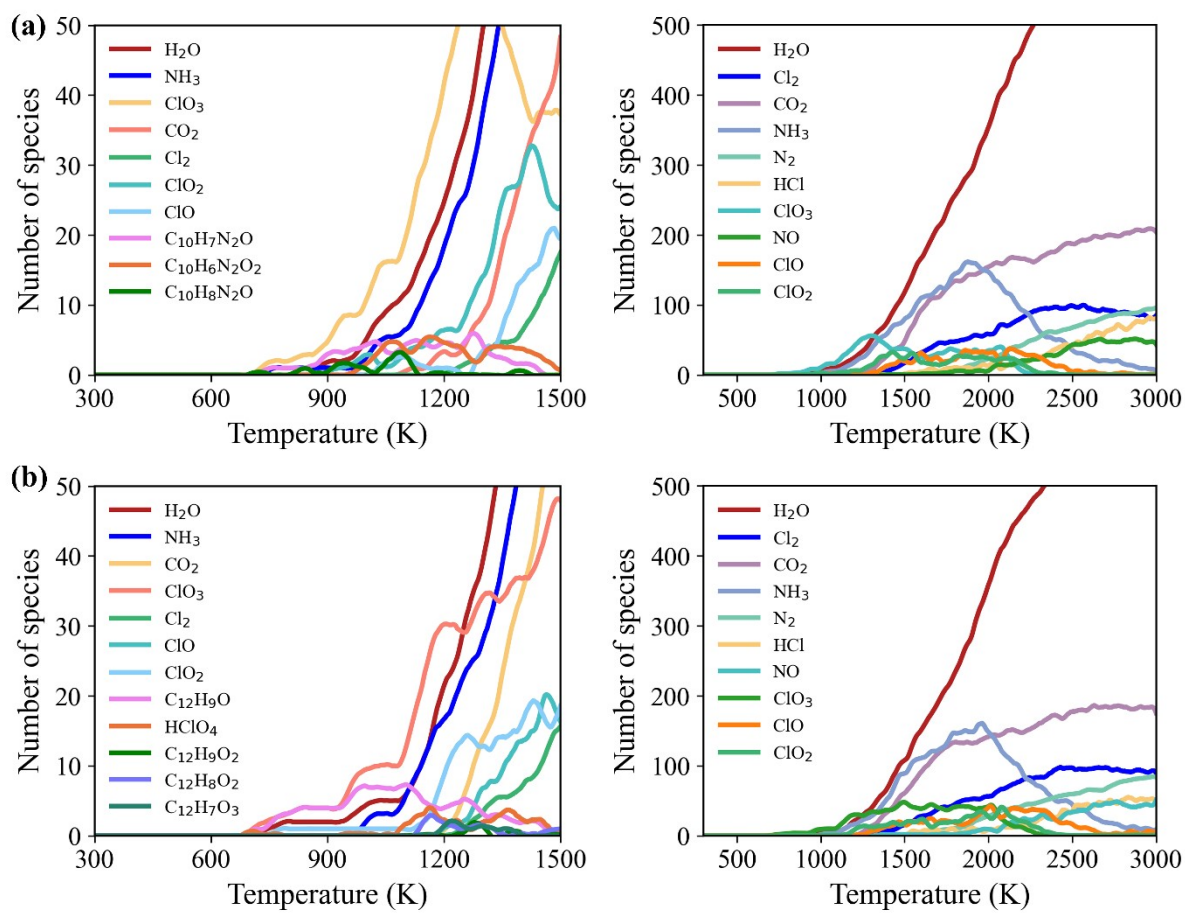
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**Fig. S1.** Morphology of AP and AP/BpyNO composites during heating. The C, H, N, O, and Cl atoms are represented in gray, white, blue, red, and green, respectively.





**Figure S4** Initial decomposition products (left) and major gas-phase products (right) of AP/Bpy (a) and AP/Bph (b).