Supporting Information

to

Adaptive Peptide Molecule as the Promising Highly-Efficient Gas-Sensor Material: In Silico Study

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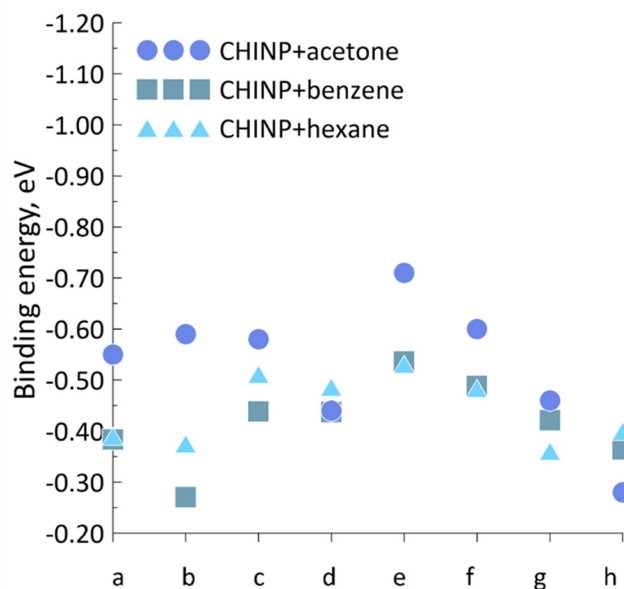
Figure S1. The values of the binding energy of the CIHNP+acetone, CIHNP+benzene, CIHNP+hexane systems depending on acetone's approaching a certain local center.
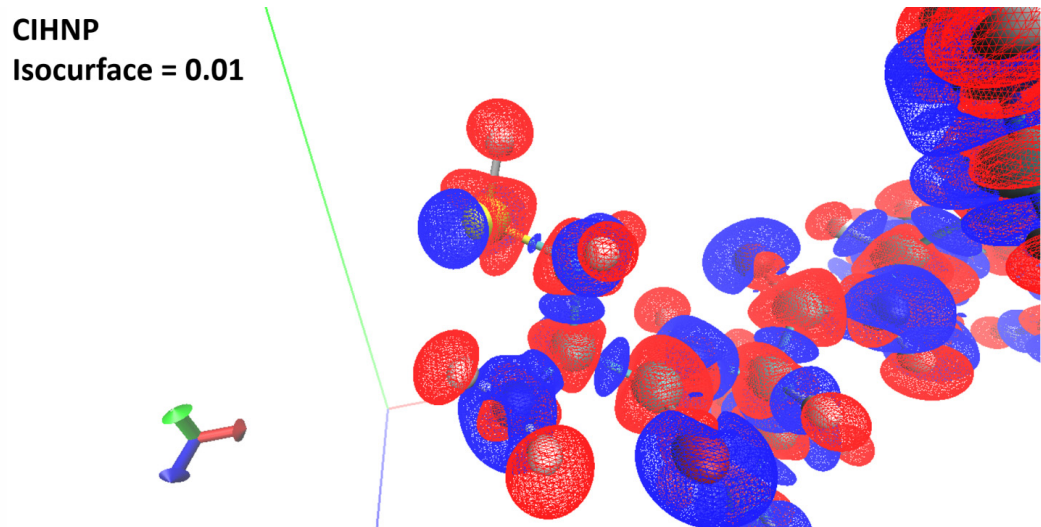
CIHNP
Isocurface = 0.01

Figure S2. The electron density of the CIHNP peptide. The areas of positive charge are marked in red, and the areas of negative charge are marked in blue. Isosurfaces of 0.01 atomic units.