Application of Spin-Ratio Scaled MP2 for the prediction of intermolecular interactions in chemical systems

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Supplementary Information
Table S1. $c_{OS}$ and $c_{SS}$ coefficients in the SRS-MP2 method with best performing basis sets, cc-pVTZ and cc-pVQZ.

<table>
<thead>
<tr>
<th>Basis set</th>
<th>$\varepsilon_{cd}$</th>
<th>$c_{OS}$</th>
<th>$c_{SS}$</th>
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<td>cc-pVTZ</td>
<td>$\geq 1$</td>
<td>1.640</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$&lt; 1$</td>
<td>0.660</td>
<td>1.140</td>
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<tr>
<td>cc-pVQZ</td>
<td>$\geq 1$</td>
<td>1.689</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$&lt; 1$</td>
<td>0.671</td>
<td>1.119</td>
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Table S2. Error statistics for SRS-MP2/cc-pVQZ in kJ mol$^{-1}$.

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<tr>
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<th>MAE$^{[a]}$</th>
<th>SD$^{[b]}$</th>
<th>Min</th>
<th>Max</th>
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<tbody>
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<td>HBIL</td>
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<td>-1.2</td>
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<td>1.4</td>
<td>-2.0</td>
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[a] Mean Absolute Error, [b] Standard Deviation

Table S3. Percentage error statistics for SRS-MP2/cc-pVQZ.

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<th>Max</th>
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</thead>
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<td>R-IL</td>
<td>9.7</td>
<td>5.9</td>
<td>28.8</td>
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<td>3.8</td>
<td>2.1</td>
<td>6.9</td>
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Figure S1. Ratio distributions for the different datasets.

Figure S2. Error distributions for SRS-MP2 and original MP2 methods using the cc-pVQZ basis set across different datasets.
Table S4. CCSD(T)/CBS interaction correlation energies for the different datasets in kJ mol\(^{-1}\).

<table>
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<tr>
<th>Dataset</th>
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<th>Max</th>
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<td>HBIL</td>
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Figure S3. Percentage error distributions for SRS-MP2 and original MP2 methods using the cc-pVTZ basis set across different datasets.
Table S5. Error statistics (all numbers are in kJ mol$^{-1}$) of MP2, SCS-MP2, SCS(MI), SCSN and SRS-MP2 for cc-pVTZ and cc-pVQZ basis sets, with cc-pVTZ used for SCSN. Error statistics for MP2/CBS are given for comparison.

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<th>Basis set</th>
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<th>Max</th>
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<td>1.23</td>
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<td>-1.97</td>
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Figure S4. Comparison of SCS-MP2, SCS(MI) and SRS-MP2 performance for the four datasets studied for cc-pVQZ basis set, except SCSN, which is only available for aug-cc-pVTZ. SCS-MP2, SCS(MI) and SCSN used counterpoise corrected energies. The following scaling coefficients were used: 1) $c_{OS} = 1.2$ and $c_{SS} = 1/3$ for SCS-MP2; 2) $c_{OS} = 0.31$ and $c_{SS} = 1.46$ for SCS(MI).
Table S5. Error statistics (all numbers are in kJ mol\(^{-1}\)) of the SRS-MP2 for all basis sets and all Separations for the S66x8 dataset.

<table>
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<th>Basis set</th>
<th>Separation</th>
<th>Mean(^1)</th>
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<th>Min</th>
<th>Max</th>
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<td>0.91</td>
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