

## Supplementary Material for the manuscript

### Contributions to Ionic Activity Coefficients: A Review and Comparison of Equations of State with Molecular Simulations

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**Part 1: Comparison between Explicit Molecular Simulations and eSAFT-VR Mie**

**Part 2: Comparison between Explicit Molecular Simulations and ePPC-SAFT**

## **Part 1: Comparison between Explicit Molecular Simulations and eSAFT-VR Mie**

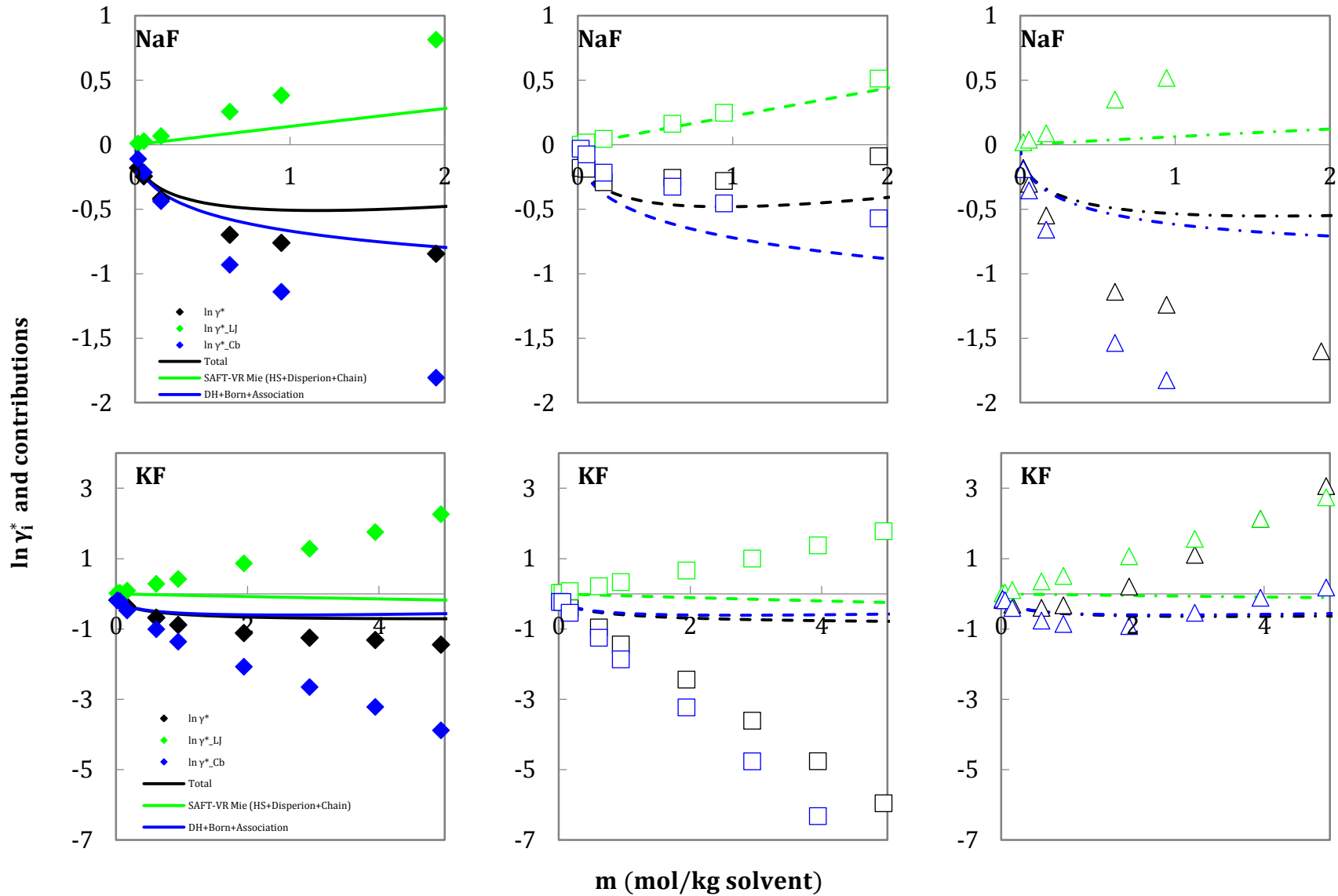


Figure S1.  $\ln \gamma_i^*$  and contribution of the various terms from explicit molecular simulation and eSAFT-VR Mie (constant). Points are explicit molecular simulations, lines are eSAFT-VR Mie calculations using the relative permittivity of the solvent.

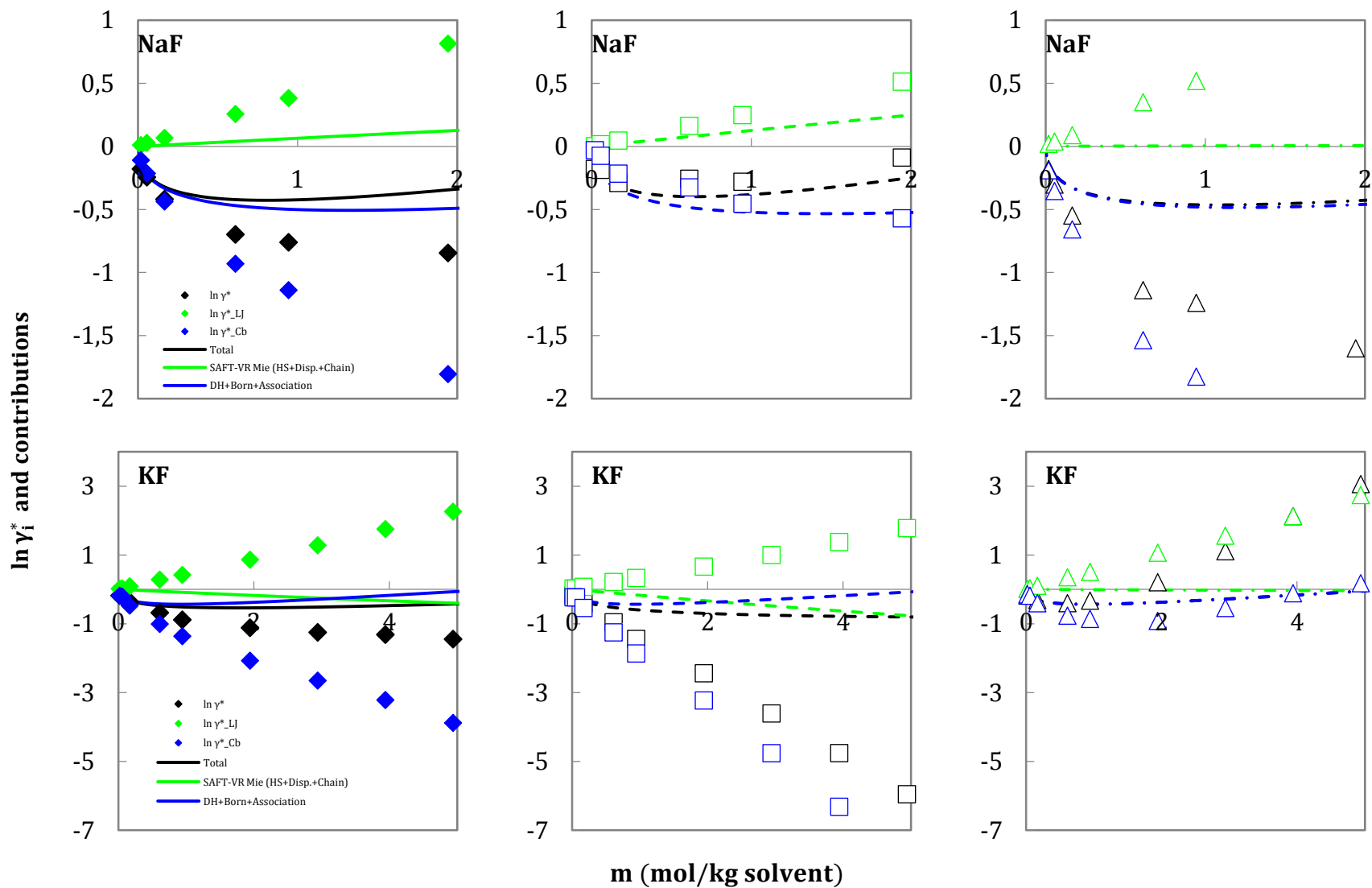


Figure S2.  $\ln \gamma_i^*$  and contribution of the various terms from explicit molecular simulation and eSAFT-VR Mie (MFMR). Points are explicit molecular simulations, lines are eSAFT-VR Mie calculations using the MFMR.

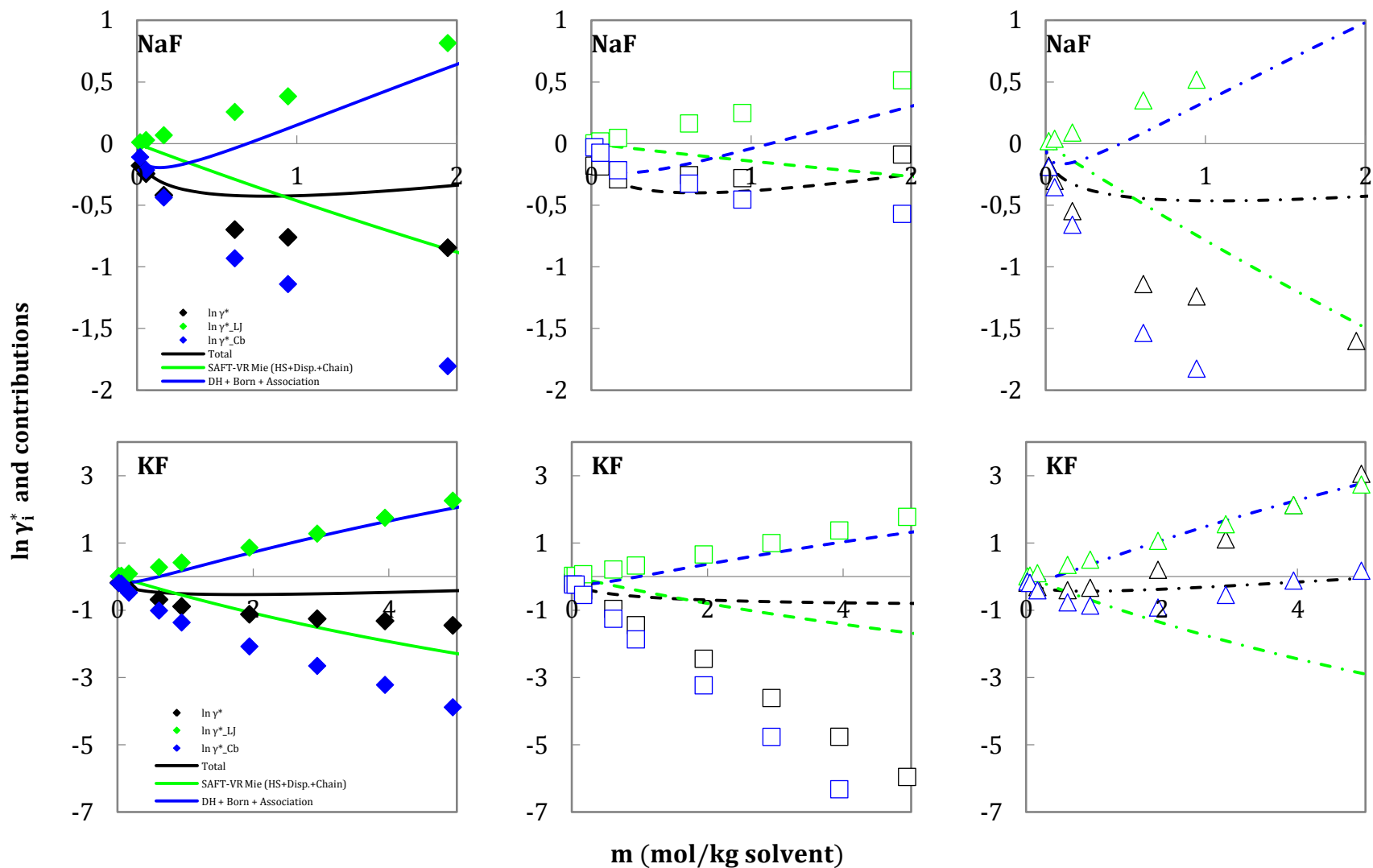


Figure S3.  $\ln \gamma_i^*$  and contribution of the various terms from explicit molecular simulation and eSAFT-VR Mie (Zuber et al.). Points are explicit molecular simulations, lines are eSAFT-VR Mie calculations using the Zuber et al..

## **Part 2: Comparison between Explicit Molecular Simulations and ePPC-SAFT**

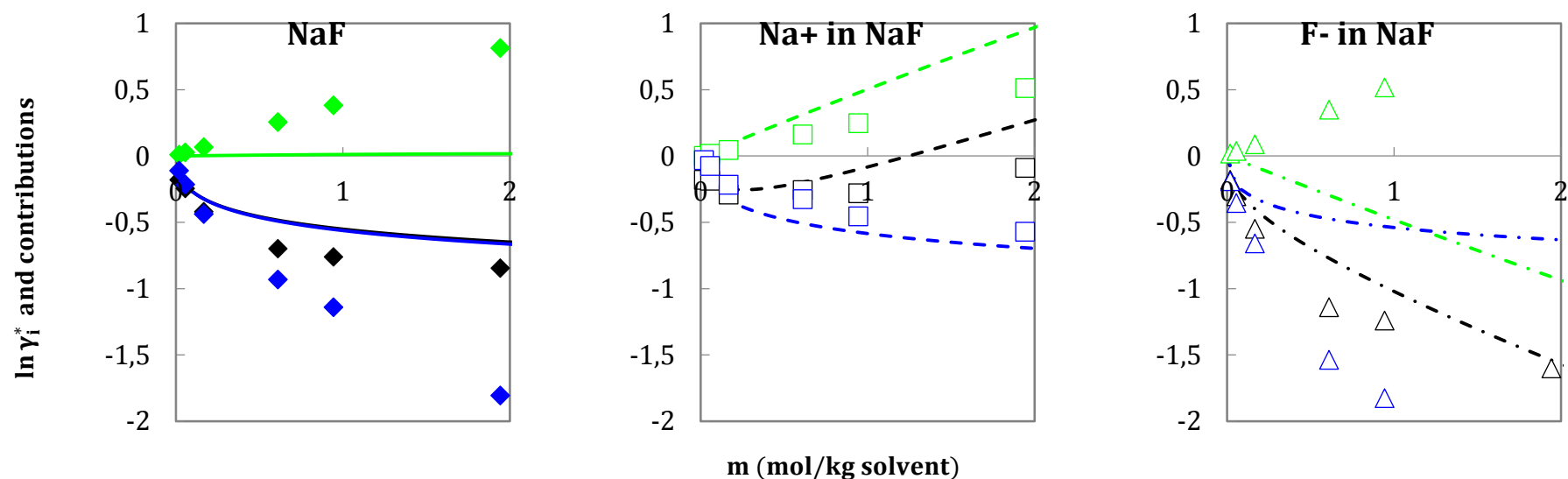


Figure S4.  $\ln \gamma_i^*$  and contributions of the various terms from explicit molecular simulation and ePPC-SAFT for NaF. Points are explicit molecular simulations. Lines are ePPC-SAFT calculations. Green points are LJ contributions. Blue points are Coulombic contributions. Blue lines are the MSA and Born contributions. Green lines are the other contributions. Black points and lines are the total  $\ln \gamma_i^*$ .

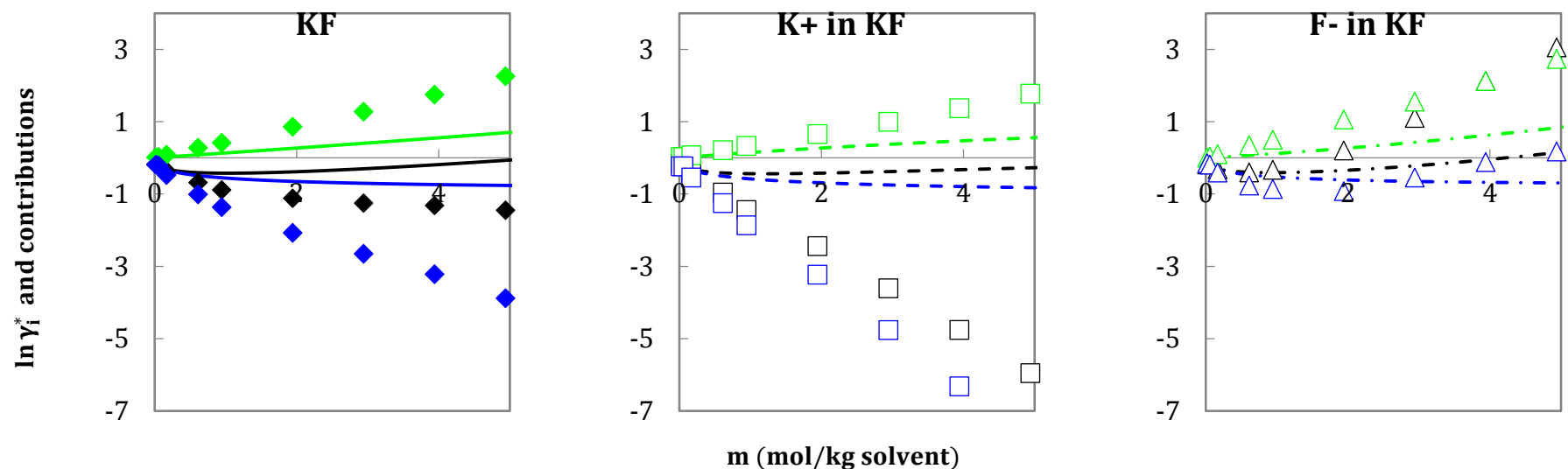


Figure S5.  $\ln \gamma_i^*$  and contributions of the various terms from explicit molecular simulation and ePPC-SAFT for KF. Points are explicit molecular simulations. Lines are ePPC-SAFT calculations. Green points are LJ contributions. Blue points are Coulombic contributions. Blue lines are the MSA and Born contributions. Green lines are the other contributions. Black points and lines are the total  $\ln \gamma_i^*$ .



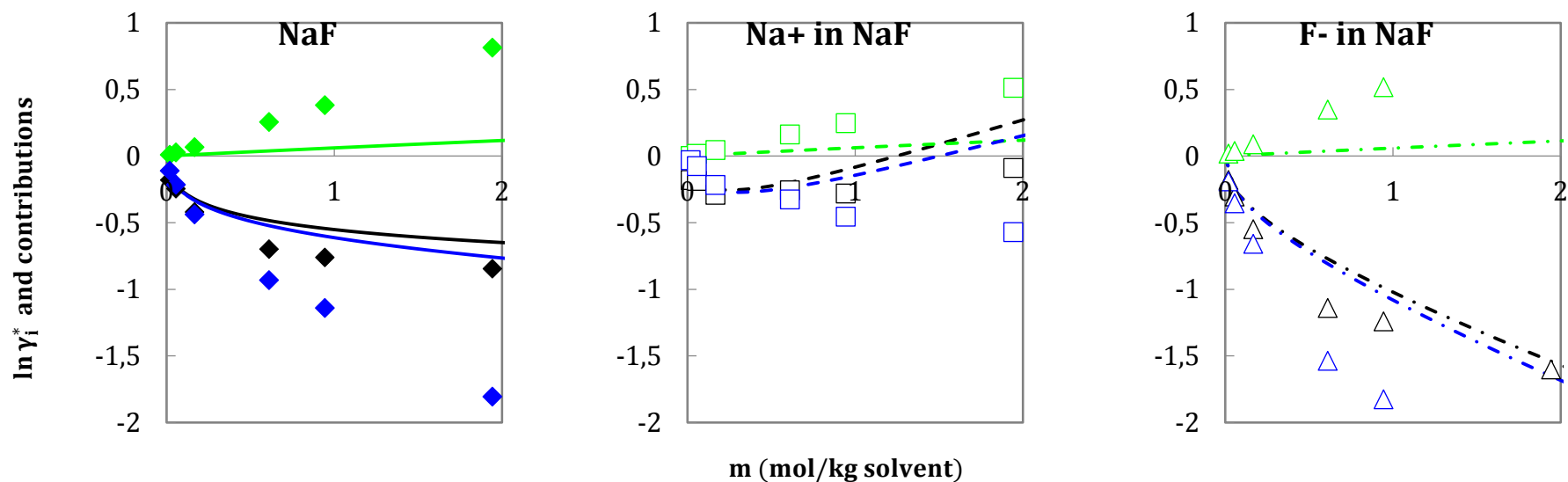


Figure S6.  $\ln \gamma_i^*$  and contributions of the various terms from explicit molecular simulation and ePPC-SAFT for NaF. Points are explicit molecular simulations. Lines are ePPC-SAFT calculations. Green points are LJ contributions. Blue points are Coulombic contributions. Blue lines are the MSA, Born, and association contributions. Green lines are the other contributions. Black points and lines are the total  $\ln \gamma_i^*$ .

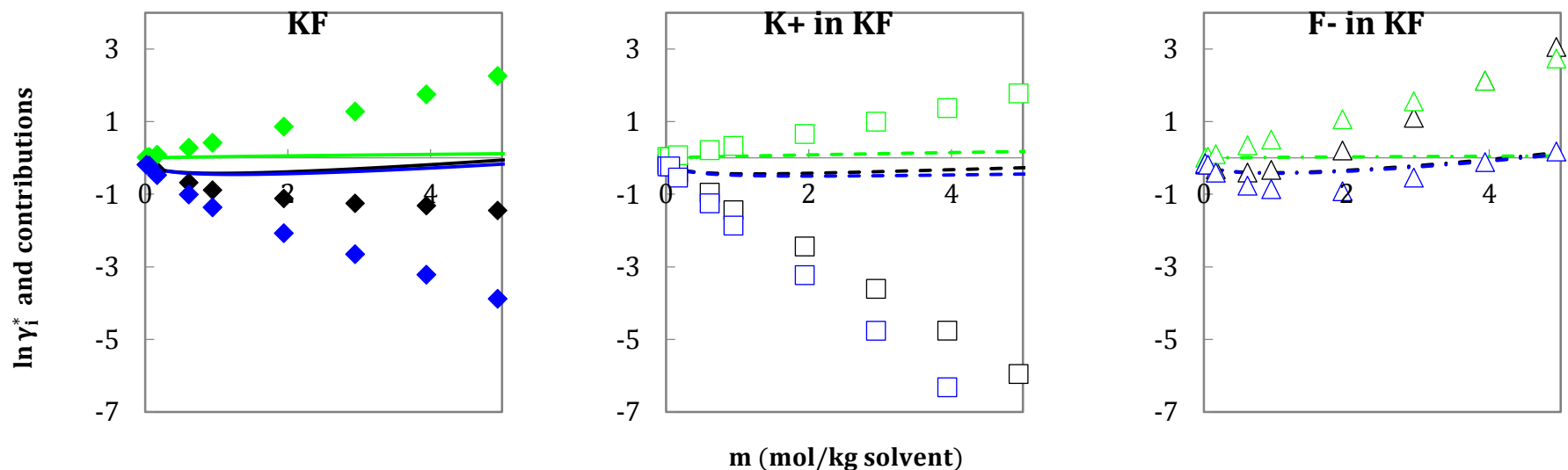


Figure S7.  $\ln \gamma_i^*$  and contributions of the various terms from explicit molecular simulation and ePPC-SAFT for KF. Points are explicit molecular simulations. Lines are ePPC-SAFT calculations. Green points are LJ contributions. Blue points are Coulombic contributions. Blue lines are the MSA, Born, and association contributions. Green lines are the other contributions. Black points and lines are the total  $\ln \gamma_i^*$ .

