Evaluation of volatile iodine trapping in presence of contaminants:

a periodic DFT study on cation exchanged-faujasite : Supporting Information

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Table S1: Summary of thermodynamic calculations for Ag-exchanged faujasite zeolite.
$H_{corr} = \Delta H - \Delta E$ is the difference between adsorption enthalpy at a finite temperature and adsorption energy at 0K.
$H_{corr} = \Delta ZPVE + \Delta H_{vib} + \Delta H_{trans} + \Delta H_{rot}$
All terms are explicated in Section 2.3 of the manuscript.

	ΔE (kJ/mol)	**T**	**ΔZPVE (kJ/mol)**	**ΔH vib (kJ/mol)**	**ΔH trans (kJ/mol)**	**ΔH rot (kJ/mol)**	**H corr**	**ΔH (kJ/mol)**
Ag-CH_3I	**-117.7**	298.15	2.7	12.9	-6.2	-3.7	5.7	**-112.0**
		373	2.7	16.5	-7.8	-4.7	6.9	**-110.8**
		523	2.7	23.9	-10.9	-6.5	9.3	**-108.4**
Ag-I_2	**-107.7**	298.15	1.55	11.3	-6.2	-2.5	4.2	**-103.5**
		373	1.55	14.4	-7.8	-3.1	5.1	**-102.6**
		523	1.55	20.6	-10.9	-4.3	6.9	**-100.8**
Ag-H_2O	**-70.0**	298.15	10.4	7.1	-6.2	-3.7	7.6	**-62.4**
		373	10.4	10.1	-7.8	-4.7	8.1	**-61.9**
		523	10.4	16.6	-10.9	-6.5	9.7	**-60.3**
Ag-CO	**-114.4**	298.15	6.53	7.7	-6.2	-2.5	5.5	**-108.9**
		373	6.53	10.5	-7.8	-3.1	6.1	**-108.3**
		523	6.53	16.3	-10.9	-4.3	7.6	**-106.8**
Ag-NO	**-77.8**	298.15	4.81	8.4	-6.2	-2.5	4.5	**-73.3**
		373	4.81	11.3	-7.8	-3.1	5.3	**-72.5**
		523	4.81	17.3	-10.9	-4.3	6.9	**-70.9**
Ag-CH_3Cl	**-82.7**	298.15	3.40	12.3	-6.2	-3.7	5.8	**-76.9**
		373	3.40	16.0	-7.8	-4.7	7.0	**-75.7**
		523	3.40	23.4	-10.9	-6.5	9.4	**-73.3**
Ag-Cl_2	**-59.6**	298.15	2.16	10.5	-6.2	-2.5	4.0	**-55.6**
		373	2.16	13.6	-7.8	-3.1	4.9	**-54.7**
		523	2.16	19.8	-10.9	-4.3	6.7	**-52.9**