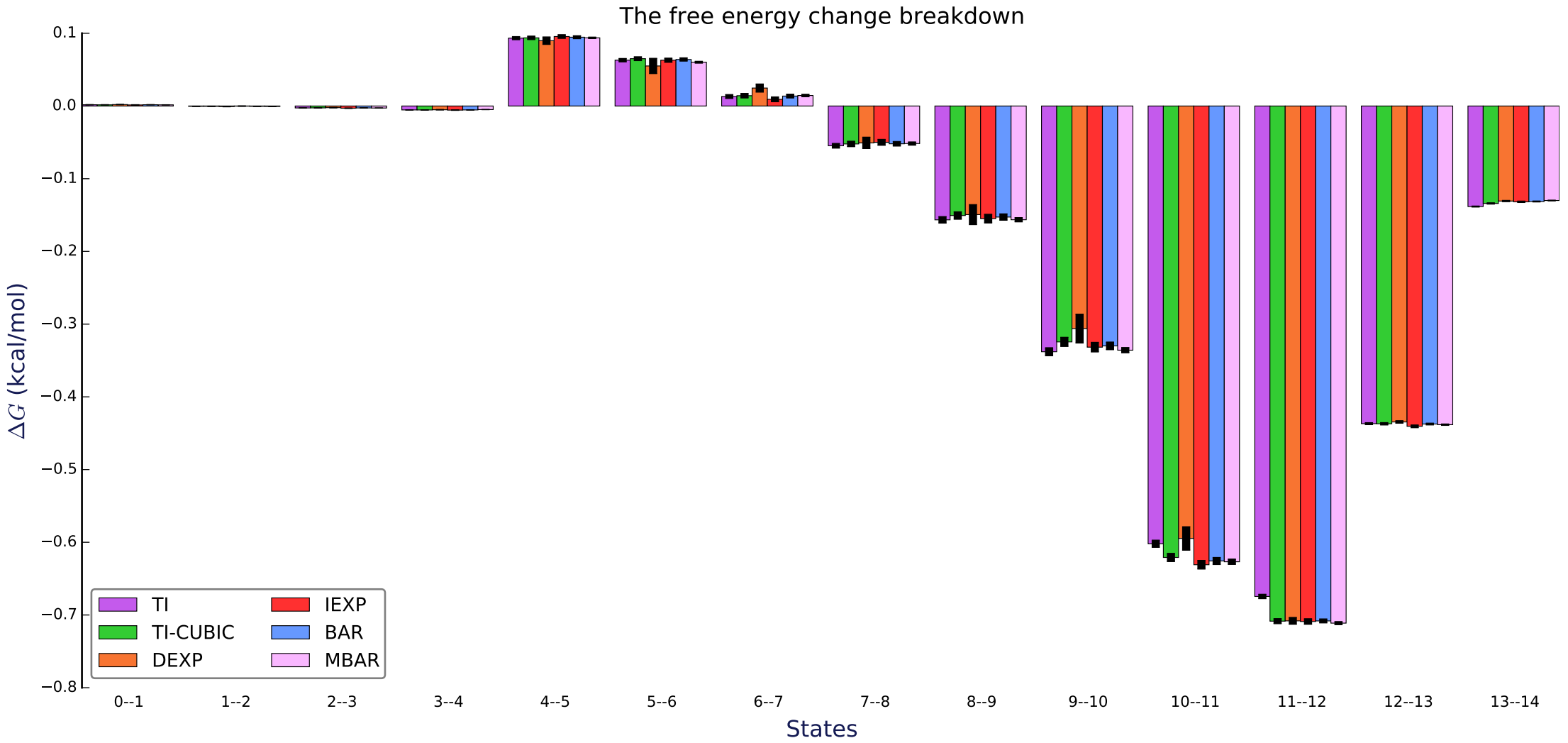
The free energy change breakdown
0.1
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
ΔG (kcal/mol)
TI
TI-CUBIC
DEXP
IEXP
BAR
MBAR
0--1
1--2
2--3
3--4
4--5
5--6
6--7
7--8
8--9
9--10
10--11
11--12
12--13
13--14
States