

% Relative deviation

40

30

20

10

0

-10

-20

—●—

GKS-spRPA

—▼—

HF

—●—

PBE

—▲—

PBE0

—■—

MP2

H

Be

Be₂

Na

LiH

Li₂

HF

H₂O

CN

N₂

CO

HCN

F₂

CH₃F

NaLi

O₂

CH₂O

CH₃NH₂

LiK

CO₂

O₃

(CH₃)₂NH

(CH₃)₃N

CH₃Br

CCl₄