

(a)

Ground truth
(Optimal structure)

SchNet

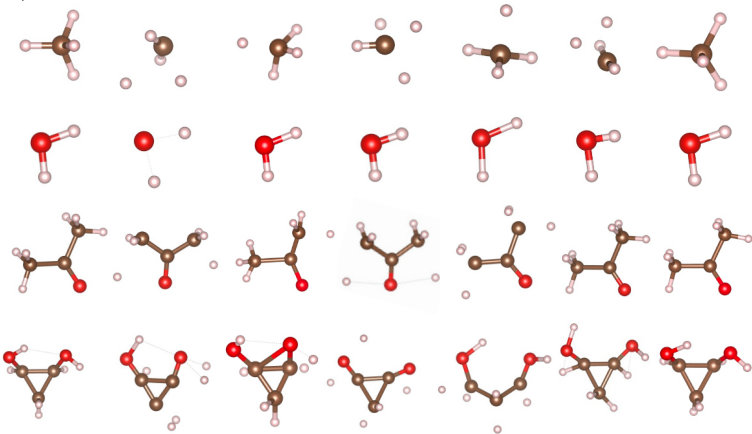
ForceNet

DimeNet

MXMNet

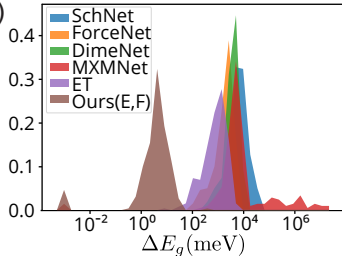
ET

Ours



(b)

Probability



(c)

Probability

