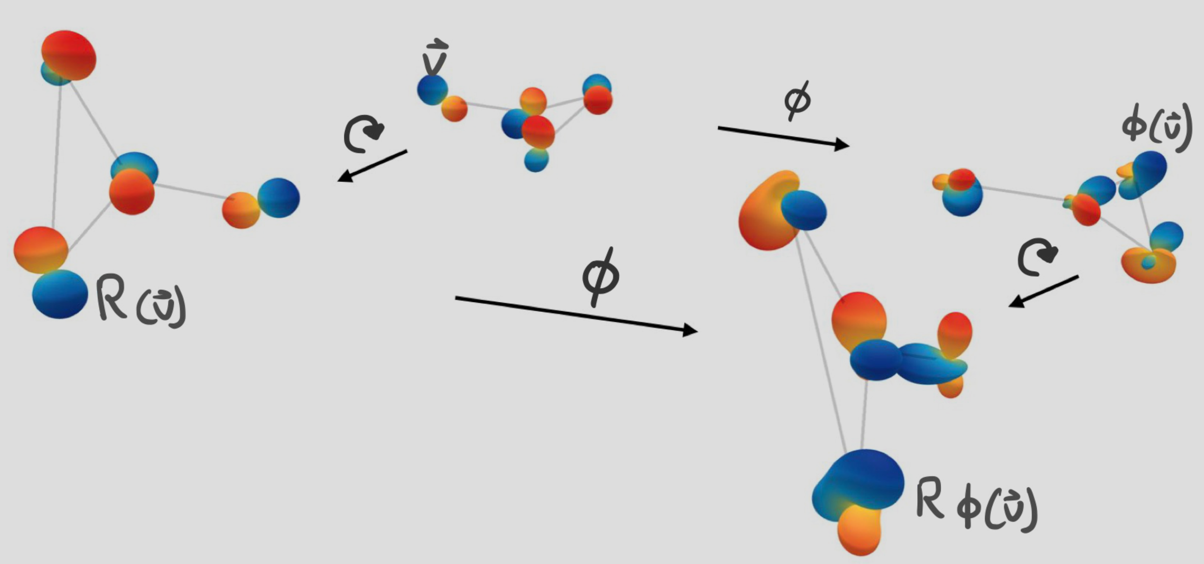
I fpn fusjd Coe R i z tjdbm Svbouujuj f t Kn qspwf G*3+ Gr vjwbsjbou O f t tbh f Rbt tjoh

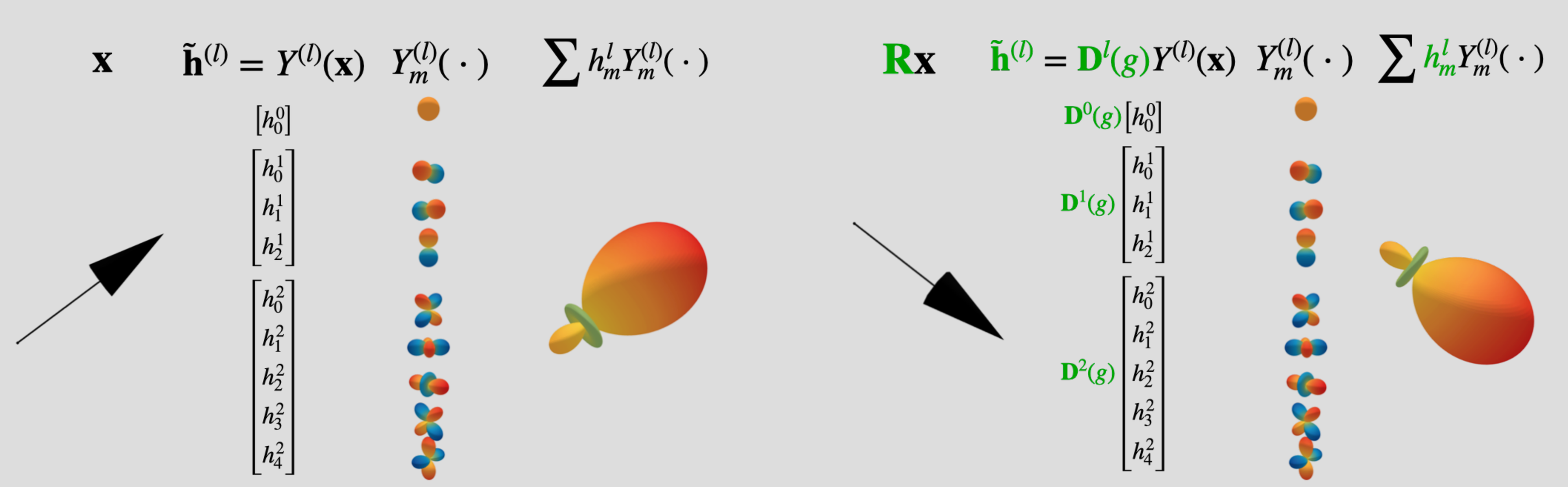
Lpiboof t Dsboetufuufs,[34] Tpc Jf t t fmjo l,[3] Gmjt f wbo e f s Rpm[3] Gsj l Df l l fst[3] Oby X fmjoh[3]

[3]Vojwfstjuz pg Cn tufseb n [4]Lp i boo f t Mf qmfs Vojwfstjuz Njo{

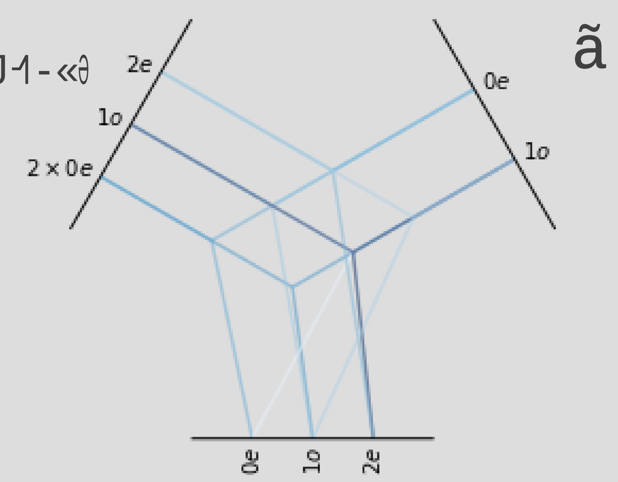
Wfdups/wbmv f e jogps n bujpo



%uf fsbcmf gfbuvsf t. tuf fsbcmf wfdups tqbdf t. tuf fsbcmf ONRt



%uf fsbcmf G*3+ Gr vjwbsjbou I sbq i P f vsbm P fuxpsl t *%G I PPt+



$$\tilde{m}_{ij} = \varphi_m\left(\tilde{f}_i, \tilde{f}_j, \underbrace{\|x_j - x_i\|^2}_{\tilde{h}_{ij}}, \tilde{a}_{ij}\right); \quad \tilde{f}_i = \varphi_f\left(\tilde{f}_i, \underbrace{\sum_{j \in N(i)} \tilde{m}_{ij}}_{\tilde{h}_i}, \tilde{a}_i\right)$$

Ppo/mjo f bs wt mjo f bs dpowpmvujpo

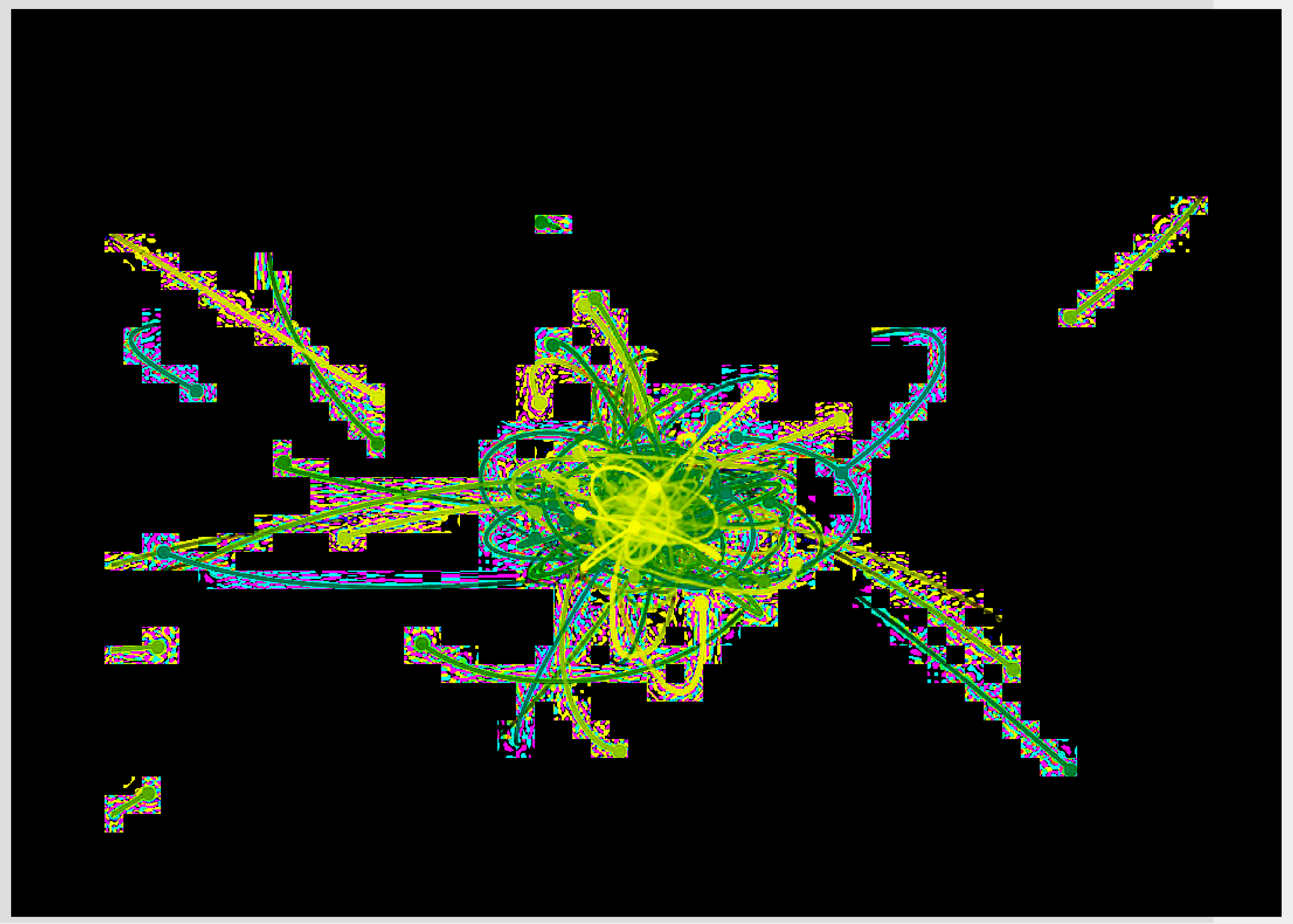
			Task / Units	α (bohr³)	Δε (meV)	ε_HOMO (meV)	ε_LUMO (meV)	μ (D)	C_v (cal/mol K)
non-linear		no geometry	NMP	.092	69	43	38	.030	.040
	regular	$\mathbb{R}^3$	SchNet *	.235	63	41	34	.033	.033
pseudo-linear	steerable	$\mathbb{R}^3$	Cormorant	.085	61	34	38	.038	.026
	steerable	$SE(3)$	L1Net	.088	68	46	35	.043	.031
	regular	G	LieConv	.084	49	30	25	.032	.038
	steerable	$SE(3)$	TFN	.223	58	40	38	.064	.101
pseudo-linear	steerable	$SE(3)$	SE(3)-Tr.	.142	53	35	33	.051	.054
non-linear	regular	$\mathbb{R}^3 \times S^2 \times \mathbb{R}^+$	DimeNet++ *	**.043**	**32**	24	19	.029	.023
non-linear	regular	$\mathbb{R}^3 \times S^2 \times \mathbb{R}^+$	SphereNet *	.046	**32**	**23**	**18**	.026	**.021**
non-linear	reguleerable?	$SE(3)$	PaiNN *	.045	45	27	20	**.012**	.024
non-linear	regular	$\mathbb{R}^3$	EGNN	.071	48	29	25	.029	.031
non-linear	steerable	$SE(3)$	SEGNN (Ours)	.060	42	24	21	.023	.031

Table 2: Comparison on QM9.

P f x tuf fsbcmf bdujwbujpo gvodujpot

$$\tilde{f}_i = \varphi_f\left(\tilde{f}_i, \underbrace{\sum_{j \in N(i)} \tilde{m}_{ij}}_{\tilde{h}_i}, \tilde{a}_i\right).$$

Rfsgpsn bodf boe bqqmjdbcjmjuz



Tfgfsfodft