

Supplemental Materials: Benchmarking Various Types of Partial Atomic Charges for Classical All-Atom Simulations of Metal-Organic Frameworks

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I. SIX-LETTER NAMES FROM THE CORE2019 DATABASE FOR THE 181 MOFS

| indices | names | indices | names | indices | names |
|---------|----------|---------|----------|---------|----------|
| 001 | ABAVIJ | 051 | FEFDAX | 101 | NAKLIW |
| 002 | ADABUE | 052 | FEWTUY | 102 | NEJRUR |
| 003 | ADAXEK | 053 | FOHCIP | 103 | NEJSEC |
| 004 | AFOYOK | 054 | FUTDII | 104 | NEVVAM |
| 005 | ANOMUM | 055 | GELJAJ | 105 | NIHQI01 |
| 006 | ATIJUJ | 056 | GELVID01 | 106 | NOFHUM |
| 007 | AVAQIX | 057 | GMSIG | 107 | OCAQOY |
| 008 | AVELOD | 058 | GIZVER | 108 | OFAWEZ |
| 009 | AVEMAQ | 059 | HAJLEK | 109 | OHAQEU |
| 010 | AWAGEL | 060 | HAJLIO | 110 | OPIWEQ |
| 011 | BAHGUN01 | 061 | HAJLOU | 111 | PAPPED |
| 012 | BAHGUN04 | 062 | HAJLUA | 112 | PEFRID |
| 013 | BAHGUN | 063 | HEGJUZ | 113 | PELGOE |
| 014 | BARZAW | 064 | HEKTUO | 114 | PESTUD |
| 015 | BARZOK | 065 | HFTOG02 | 115 | PEWXUL01 |
| 016 | BASTEW | 066 | ICAGOK | 116 | PEWXUL |
| 017 | BEPVEZ | 067 | IFENYO | 117 | PEXBIF |
| 018 | BEZSIK | 068 | ILUJEF | 118 | PEYSIW |
| 019 | BIHMUC | 069 | IQUNAJ01 | 119 | PIJJOI |
| 020 | BURJOO | 070 | ISIKIF | 120 | PURJIW |
| 021 | BUSQEM | 071 | ITETEH | 121 | QEBGAH |
| 022 | BUVXOG | 072 | IVETOT | 122 | QOKCID |
| 023 | BUVYEX | 073 | IXEQIL | 123 | QOPHEI |
| 024 | BUVYIB | 074 | JASNAT | 124 | QUPJAN |
| 025 | CAHSOU | 075 | JASNEX | 125 | QUPZAC |
| 026 | CAVSUP | 076 | KANDIO | 126 | RETBEZ |
| 027 | CAXVII | 077 | KENJEU | 127 | RIBDEN |
| 028 | CAXVOO | 078 | KEVWUF | 128 | SAXFII |
| 029 | CAXVUU | 079 | KIDDOS | 129 | SETSIV |
| 030 | CAXWAB | 080 | KIFWUT | 130 | SOWYOS |
| 031 | CAXWIJ | 081 | KUXLUL | 131 | SUJQOE |
| 032 | CAYSOK | 082 | LAGHIL | 132 | SUJREV |
| 033 | CEGDUO | 083 | LAGWEX | 133 | TAGSEB |
| 034 | CESYEF01 | 084 | LEDCAA | 134 | TARVOX |
| 035 | CITXUZ | 085 | LEGGOU | 135 | TEQPAI |
| 036 | CUGLTM01 | 086 | LEPLEZ | 136 | TEQVAO |
| 037 | CUGLTM | 087 | LERNEC01 | 137 | TESHAB |
| 038 | CUVTUJ | 088 | LERNEC | 138 | TETZID |
| 039 | DAGDUL | 089 | LOLQIM | 139 | TEWGEJ01 |
| 040 | DAWBOU | 090 | LUKRUE | 140 | TIRRIW |
| 041 | DAWCAH | 091 | LUMDEC | 141 | TOLGOR |
| 042 | DAXHIV01 | 092 | LUPTAS | 142 | TUTZOX |
| 043 | DAXHIV | 093 | MABJUV01 | 143 | UBACOR |
| 044 | DAXHUH | 094 | MABKEG | 144 | UKULOB |
| 045 | DIDBEZ | 095 | MATTOR | 145 | UMELUU |
| 046 | DIZQOT | 096 | MATTUX | 146 | UNABUH01 |
| 047 | DOKHOB | 097 | MEHPAQ | 147 | UNABUH |
| 048 | EBIHII | 098 | MIZJUB | 148 | UNACIW |
| 049 | FAKGOP | 099 | MOYYIJ | 149 | UWUTIQ |
| 050 | FECZAQ | 100 | MUWQEB | 150 | VAGTAA |

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|---------|----------|
| 151 | VAQLEG |
| 152 | VONBIK |
| 153 | WAFKAQ |
| 154 | WAHMEY01 |
| 155 | WEJSAH |
| 156 | WEYMIY |
| 157 | WEZCIO |
| 158 | WODFOL |
| 159 | WOHBIF |
| 160 | WOLMUG |
| 161 | WUTBES |
| 162 | XACZEH |
| 163 | XAMDUM04 |
| 164 | XAMDUM05 |
| 165 | XAMDUM |
| 166 | XAPSOY |
| 167 | XAPYAO |
| 168 | XAWZOM |
| 169 | XEJWUG |
| 170 | XIMPOA |
| 171 | XINRAP |
| 172 | XOKHAH |
| 173 | XUCNOZ |
| 174 | XUMFIV |
| 175 | XUVHEB |
| 176 | YACHUH |
| 177 | YARSAN |
| 178 | YEZKIZ |
| 179 | YUCNEQ |
| 180 | YUWKIL |
| 181 | ZEDROR |

II. THE STATISTICAL AND PHYSICAL INFORMATION OF THE 181 MOFS

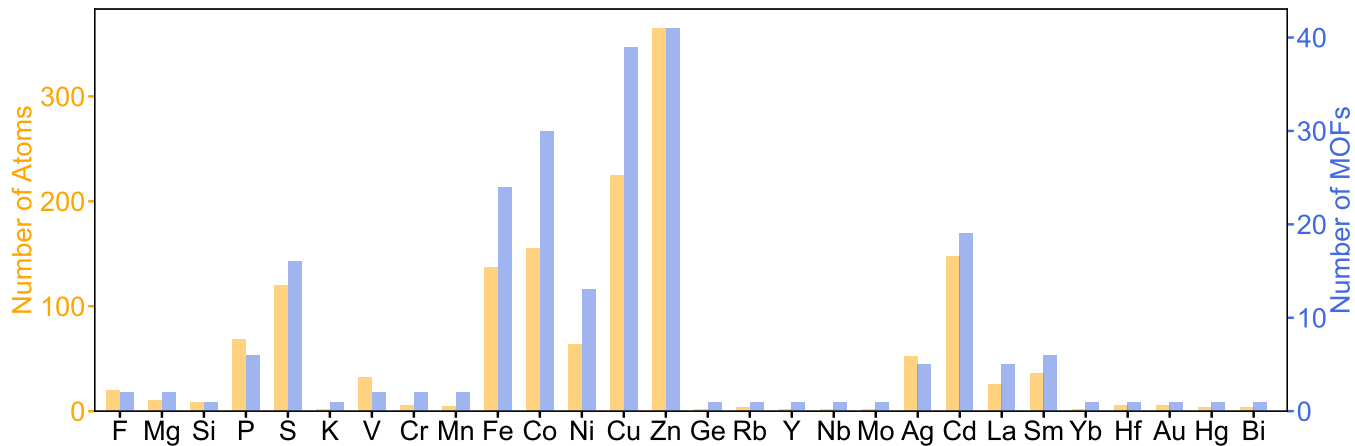


FIG. S1: The frequencies of the different elements in the 181 MOFs (orange bars) and the number of MOFs containing each element (blue bars). H, C, N and O are excluded from the graph, and their counts are 9977, 13873, 2418, and 4462, respectively.

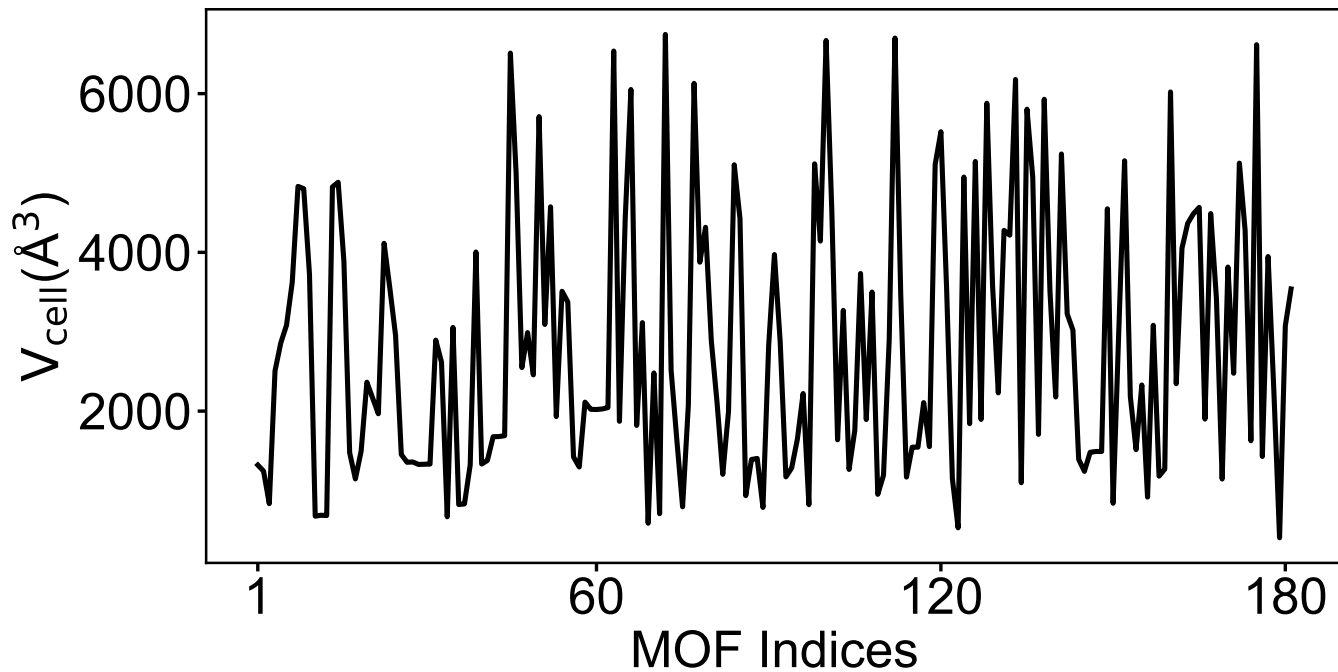


FIG. S2: The primitive cell volumes V_{cell} versus the MOF indices.

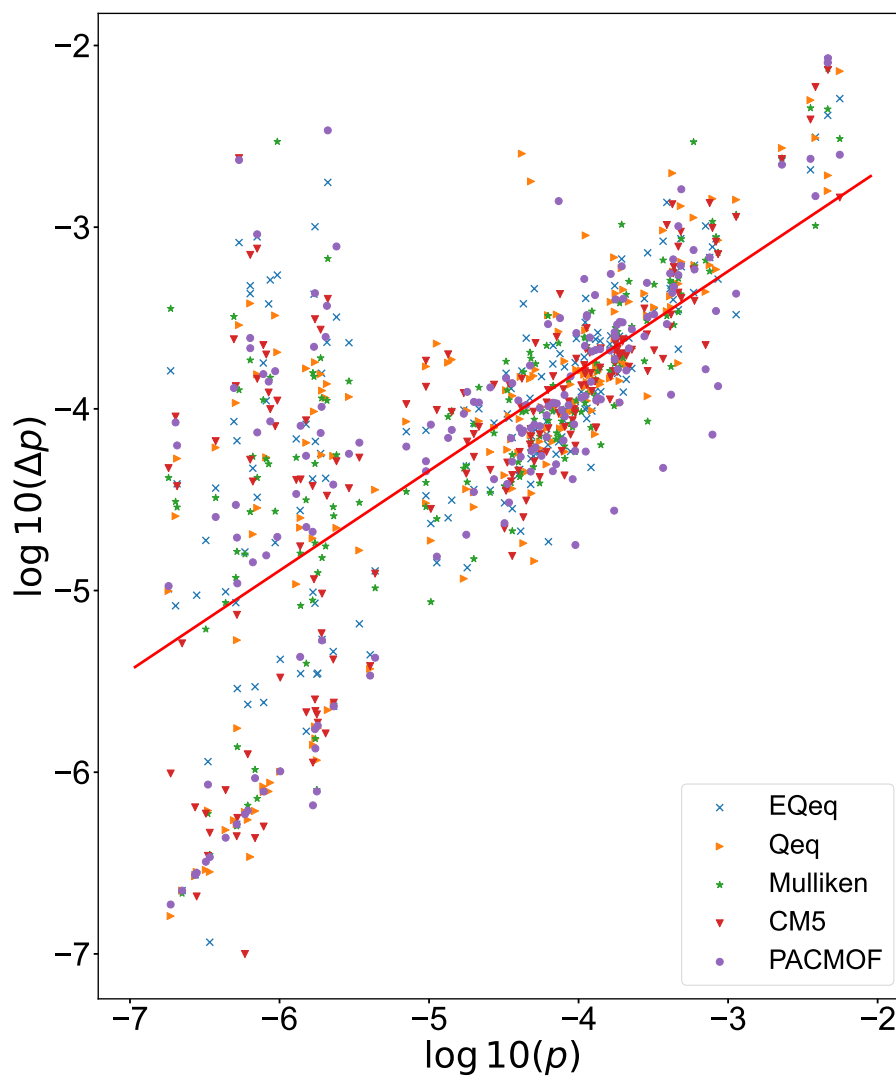


FIG. S3: The calculated Δp for the 181 MOFs are plotted against p , where points based on different charges are labelled using the distinct markers. All the data points are fitted to a red line, which indicates a linear correlation between $\log_{10}(p)$ and $\log_{10}(\Delta p)$ when $p > 10^{-4} e\text{\AA}^{-2}$.

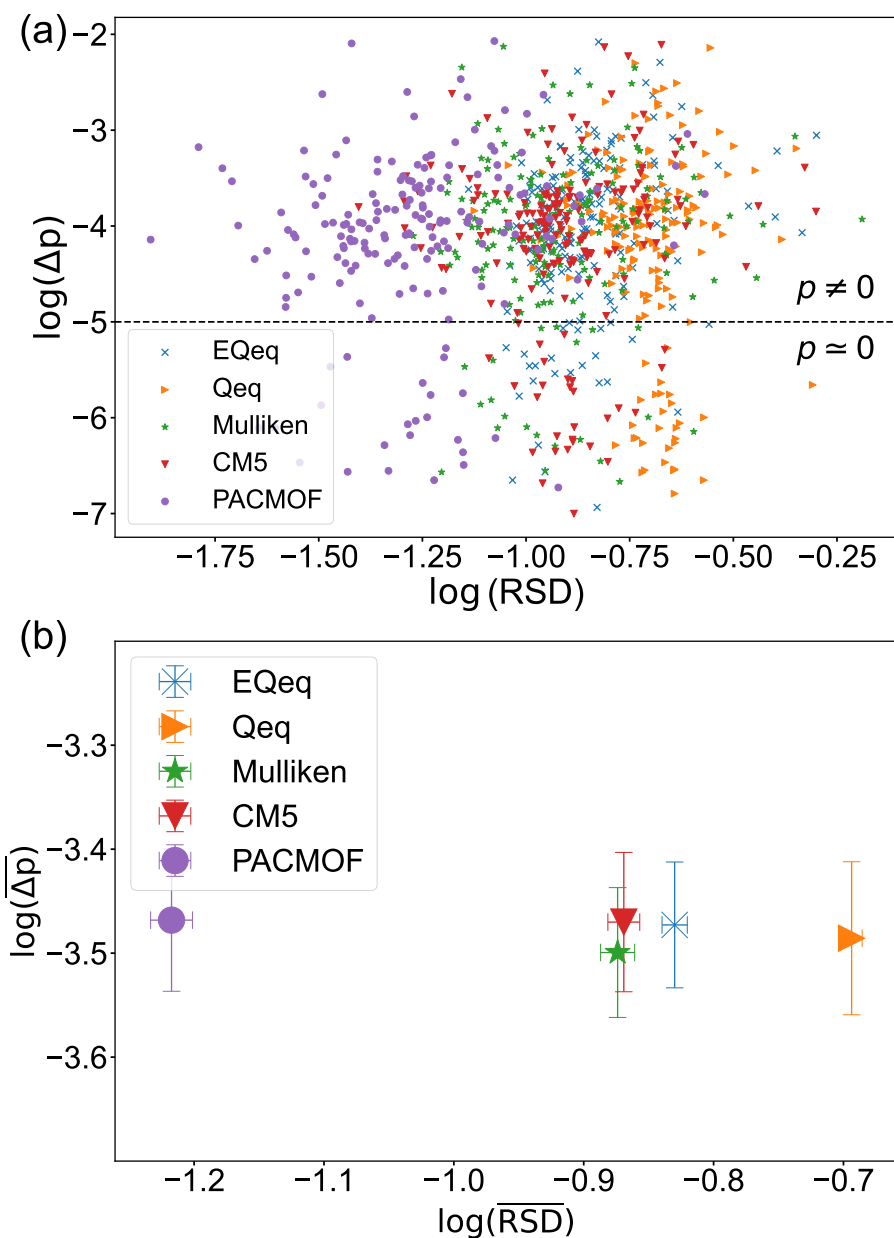
III. $|\Delta p|$ VERSUS RSD

FIG. S4: The calculated Δp for the 181 MOFs are plotted against RSD in (a), where points based on different charges are labelled using distinct markers. The points in (b) locate at the coordinates of $(\overline{\Delta p}, \overline{RSD})$ based on the five charge types, and the horizontal and the vertical bars at each point are standard error of Δp and RSD, respectively.