

## SUPPLEMENTARY INFORMATION

Coordinates of atoms for the optimized CeO<sub>2</sub>/rGO and CeO<sub>2</sub>/GP structures

### CeO<sub>2</sub>/rGO

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 28.639287800 | 14.168415330 | 11.642620670 |
| 6 | 32.412221800 | 14.824304330 | 11.677044670 |
| 6 | 24.904646800 | 14.851450330 | 11.254708670 |
| 6 | 36.164394800 | 14.201510330 | 11.534610670 |
| 6 | 24.913601800 | 16.391024330 | 11.146870670 |
| 6 | 29.930288800 | 14.880360330 | 11.505855670 |
| 6 | 31.127566800 | 14.115076330 | 11.520287670 |
| 6 | 27.383866800 | 14.891229330 | 11.333439670 |
| 6 | 33.690233800 | 14.114588330 | 11.476773670 |
| 6 | 28.638287800 | 12.621335330 | 11.456500670 |
| 6 | 21.153901800 | 14.236384330 | 11.378231670 |
| 6 | 21.187373800 | 17.115181330 | 11.370681670 |
| 6 | 26.191146800 | 14.137152330 | 11.192416670 |
| 6 | 17.413498800 | 16.483746330 | 11.407061670 |
| 6 | 32.408057800 | 16.370853330 | 11.377285670 |
| 6 | 36.163870800 | 12.614580330 | 11.350727670 |
| 6 | 28.661545800 | 17.036348330 | 11.327389670 |
| 6 | 22.431658800 | 14.944795330 | 11.211882670 |
| 6 | 34.879629800 | 14.879990330 | 11.379237670 |
| 6 | 27.388907800 | 16.303228330 | 11.216584670 |
| 6 | 32.408115800 | 11.973547330 | 11.327642670 |
| 6 | 23.615136800 | 14.170927330 | 11.106945670 |
| 6 | 22.439094800 | 16.358427330 | 11.147224670 |
| 6 | 31.125801800 | 12.707247330 | 11.337524670 |
| 6 | 19.894821800 | 16.402613330 | 11.287564670 |
| 6 | 29.936378800 | 16.287195330 | 11.308097670 |
| 6 | 33.691414800 | 12.706365330 | 11.304103670 |

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| 6 | 17.413978800 | 14.923373330 | 11.253819670 |
| 6 | 19.885318800 | 14.982897330 | 11.236233670 |
| 6 | 18.705088800 | 17.170784330 | 11.216039670 |
| 6 | 26.209821800 | 17.051725330 | 10.972590670 |
| 6 | 23.634726800 | 17.089010330 | 10.943527670 |
| 6 | 37.423571800 | 14.896495330 | 11.203200670 |
| 6 | 26.177349800 | 12.736839330 | 11.098199670 |
| 6 | 38.617819800 | 14.153980330 | 11.170405670 |
| 6 | 13.672684800 | 17.115665330 | 11.112541670 |
| 6 | 16.144534800 | 17.183907330 | 11.121325670 |
| 6 | 24.888388800 | 12.032188330 | 11.036932670 |
| 6 | 29.928083800 | 11.971049330 | 11.133795670 |
| 6 | 34.879967800 | 11.984448330 | 11.047168670 |
| 6 | 21.201734800 | 18.637068330 | 11.047777670 |
| 6 | 23.618512800 | 12.776014330 | 10.950388670 |
| 6 | 14.957511800 | 16.420629330 | 11.041616670 |
| 6 | 27.375224800 | 11.982631330 | 11.023212670 |
| 6 | 31.126197800 | 17.007272330 | 11.053357670 |
| 6 | 18.698345800 | 14.247169330 | 11.032486670 |
| 6 | 21.150568800 | 12.721571330 | 11.022071670 |
| 6 | 34.871159800 | 16.260564330 | 11.019758670 |
| 6 | 38.639787800 | 12.741260330 | 10.990120670 |
| 6 | 18.720039800 | 18.561323330 | 10.925260670 |
| 6 | 13.684891800 | 18.688799330 | 10.872051670 |
| 6 | 37.406584800 | 12.012855330 | 10.878990670 |
| 6 | 17.447580800 | 19.306026330 | 10.875339670 |
| 6 | 16.156240800 | 18.587158330 | 10.881857670 |
| 6 | 33.651957800 | 16.965349330 | 10.871891670 |
| 6 | 23.656552800 | 18.475245330 | 10.718206670 |
| 6 | 37.353567800 | 16.247002330 | 10.837325670 |

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| 6 | 14.961088800 | 15.006171330 | 10.814620670 |
| 6 | 28.672856800 | 18.499533330 | 10.784138670 |
| 6 | 16.179670800 | 14.282410330 | 10.782856670 |
| 6 | 12.431444800 | 16.410578330 | 10.775767670 |
| 6 | 26.212434800 | 18.419705330 | 10.645841670 |
| 6 | 32.403704800 | 10.541369330 | 10.698510670 |
| 6 | 24.945484800 | 19.167343330 | 10.617080670 |
| 6 | 39.847220800 | 12.064744330 | 10.705178670 |
| 6 | 22.426771800 | 12.073645330 | 10.693136670 |
| 6 | 36.117978800 | 16.926815330 | 10.683582670 |
| 6 | 19.921809800 | 19.268404330 | 10.669691670 |
| 6 | 11.225261800 | 17.134770330 | 10.622902670 |
| 6 | 14.978724800 | 19.304420330 | 10.579922670 |
| 6 | 22.467251800 | 19.223685330 | 10.561150670 |
| 6 | 29.934816800 | 10.658516330 | 10.585712670 |
| 6 | 18.702961800 | 12.886526330 | 10.582712670 |
| 6 | 12.475381800 | 15.012652330 | 10.563331670 |
| 6 | 13.727208800 | 14.316920330 | 10.530932670 |
| 6 | 27.374813800 | 10.672725330 | 10.489993670 |
| 6 | 9.981852800  | 16.406983330 | 10.479037670 |
| 6 | 24.900344800 | 10.598796330 | 10.440368670 |
| 6 | 34.880953800 | 10.691607330 | 10.424696670 |
| 6 | 19.917111800 | 12.161806330 | 10.461158670 |
| 6 | 11.231256800 | 18.560977330 | 10.413739670 |
| 6 | 31.128947800 | 18.302936330 | 10.438557670 |
| 6 | 28.653030800 | 9.941653330  | 10.384215670 |
| 6 | 10.020235800 | 14.998645330 | 10.387961670 |
| 6 | 27.406626800 | 19.094392330 | 10.341515670 |
| 6 | 12.452644800 | 19.282760330 | 10.351934670 |
| 6 | 8.771075800  | 17.122714330 | 10.341348670 |

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| 6 | 11.240507800 | 14.292278330 | 10.335496670 |
| 6 | 37.375309800 | 10.733114330 | 10.283879670 |
| 6 | 16.225123800 | 12.948611330 | 10.308574670 |
| 6 | 31.126960800 | 10.007253330 | 10.207196670 |
| 6 | 39.858627800 | 10.744758330 | 10.198087670 |
| 6 | 33.611183800 | 18.226919330 | 10.231067670 |
| 6 | 17.471856800 | 20.709127330 | 10.166323670 |
| 6 | 29.918133800 | 18.996675330 | 10.193576670 |
| 6 | 33.659824800 | 10.034834330 | 10.128899670 |
| 6 | 17.475928800 | 12.259177330 | 10.174034670 |
| 6 | 8.755864800  | 18.519995330 | 10.132625670 |
| 6 | 13.758282800 | 12.950927330 | 10.134969670 |
| 6 | 36.068228800 | 18.209110330 | 10.106258670 |
| 6 | 10.013983800 | 19.227515330 | 10.077385670 |
| 6 | 36.119044800 | 10.082909330 | 10.026484670 |
| 6 | 26.194083800 | 10.047708330 | 10.028423670 |
| 6 | 22.441822800 | 10.800371330 | 10.051434670 |
| 6 | 11.295683800 | 12.918239330 | 10.016153670 |
| 6 | 19.930222800 | 20.539322330 | 10.020993670 |
| 6 | 15.003966800 | 12.280839330 | 9.962768670  |
| 6 | 32.365604800 | 18.882702330 | 9.980881670  |
| 6 | 38.601250800 | 10.092615330 | 9.925546670  |
| 6 | 14.994097800 | 20.582935330 | 9.921783670  |
| 6 | 41.061680800 | 10.065974330 | 9.894125670  |
| 6 | 7.558797800  | 19.230863330 | 9.892510670  |
| 6 | 24.948076800 | 20.536235330 | 9.858858670  |
| 6 | 22.480605800 | 20.478079330 | 9.900051670  |
| 6 | 12.523810800 | 12.246410330 | 9.850654670  |
| 6 | 34.846895800 | 18.849852330 | 9.812359670  |
| 6 | 23.666900800 | 10.129759330 | 9.799736670  |

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|---|--------------|--------------|-------------|
| 6 | 12.504553800 | 20.576985330 | 9.773506670 |
| 6 | 19.967548800 | 10.911936330 | 9.791053670 |
| 6 | 21.215045800 | 21.204032330 | 9.726591670 |
| 6 | 10.039683800 | 20.582663330 | 9.631250670 |
| 6 | 18.746226800 | 21.177616330 | 9.614803670 |
| 6 | 16.218680800 | 21.203878330 | 9.591975670 |
| 6 | 17.506145800 | 10.962752330 | 9.582790670 |
| 6 | 7.561866800  | 20.592515330 | 9.511536670 |
| 6 | 13.765135800 | 21.207997330 | 9.526354670 |
| 6 | 28.663944800 | 8.682803330  | 9.499633670 |
| 6 | 27.404740800 | 20.282069330 | 9.545391670 |
| 6 | 21.216065800 | 10.240913330 | 9.562822670 |
| 6 | 11.288416800 | 21.235739330 | 9.421061670 |
| 6 | 15.038229800 | 10.954109330 | 9.439161670 |
| 6 | 23.663088800 | 21.036913330 | 9.372716670 |
| 6 | 31.144179800 | 8.839288330  | 9.366292670 |
| 6 | 12.581494800 | 10.919763330 | 9.368644670 |
| 6 | 8.819902800  | 21.264473330 | 9.334380670 |
| 6 | 33.636636800 | 8.858393330  | 9.333751670 |
| 6 | 41.065113800 | 8.783913330  | 9.301091670 |
| 6 | 36.108106800 | 8.841859330  | 9.321071670 |
| 6 | 29.881011800 | 20.152772330 | 9.364643670 |
| 6 | 18.751643800 | 10.310144330 | 9.340058670 |
| 6 | 38.584023800 | 8.813412330  | 9.297038670 |
| 6 | 6.360468800  | 21.311556330 | 9.254047670 |
| 6 | 16.284029800 | 10.313498330 | 9.202867670 |
| 6 | 32.344454800 | 20.088566330 | 9.218387670 |
| 6 | 26.190062800 | 20.911514330 | 9.184536670 |
| 6 | 26.203807800 | 8.896056330  | 9.174351670 |
| 6 | 13.806421800 | 10.271200330 | 9.119057670 |

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| 6 | 34.797521800 | 20.073030330 | 9.100812670 |
| 6 | 42.272594800 | 8.093081330  | 8.996125670 |
| 6 | 39.811353800 | 8.158063330  | 8.976894670 |
| 6 | 28.641428800 | 20.778726330 | 9.019936670 |
| 6 | 37.338133800 | 8.204280330  | 8.965578670 |
| 6 | 34.867865800 | 8.250464330  | 8.942475670 |
| 6 | 23.718021800 | 8.985660330  | 8.965210670 |
| 6 | 32.390864800 | 8.272303330  | 8.941353670 |
| 6 | 29.939468800 | 8.246749330  | 8.925482670 |
| 6 | 8.854109800  | 22.615989330 | 8.843733670 |
| 6 | 11.323056800 | 22.559912330 | 8.847216670 |
| 6 | 6.401359800  | 22.638950330 | 8.816144670 |
| 6 | 31.107666800 | 20.695750330 | 8.867106670 |
| 6 | 27.424114800 | 8.278571330  | 8.824244670 |
| 6 | 13.792963800 | 22.465526330 | 8.820125670 |
| 6 | 21.250960800 | 9.034810330  | 8.801632670 |
| 6 | 33.582725800 | 20.678980330 | 8.764303670 |
| 6 | 16.252770800 | 22.352276330 | 8.733141670 |
| 6 | 18.785473800 | 9.051261330  | 8.660424670 |
| 6 | 7.621329800  | 23.286262330 | 8.601157670 |
| 6 | 24.973782800 | 8.377517330  | 8.644363670 |
| 6 | 18.733464800 | 22.246738330 | 8.634873670 |
| 6 | 10.103492800 | 23.227530330 | 8.593384670 |
| 6 | 21.211431800 | 22.352875330 | 8.621211670 |
| 6 | 16.319318800 | 9.027343330  | 8.580091670 |
| 6 | 12.576420800 | 23.128325330 | 8.531219670 |
| 6 | 13.866729800 | 8.978086330  | 8.539077670 |
| 6 | 22.498676800 | 8.428800330  | 8.472174670 |
| 6 | 42.243326800 | 6.835715330  | 8.385772670 |
| 6 | 15.035543800 | 22.985792330 | 8.397591670 |

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| 6 | 20.030466800 | 8.435307330  | 8.359140670 |
| 6 | 23.661294800 | 22.048154330 | 8.339073670 |
| 6 | 39.792062800 | 6.875636330  | 8.326347670 |
| 6 | 17.563731800 | 8.412961330  | 8.281100670 |
| 6 | 37.324061800 | 6.945249330  | 8.260380670 |
| 6 | 17.494840800 | 22.824099330 | 8.252834670 |
| 6 | 15.086709800 | 8.359783330  | 8.242010670 |
| 6 | 26.151403800 | 21.937153330 | 8.185411670 |
| 6 | 34.860192800 | 7.028438330  | 8.172879670 |
| 6 | 32.395318800 | 7.108741330  | 8.089681670 |
| 6 | 28.619841800 | 21.884046330 | 8.098090670 |
| 6 | 41.029839800 | 6.230245330  | 8.046702670 |
| 6 | 19.927082800 | 22.684655330 | 8.045700670 |
| 6 | 31.082908800 | 21.860701330 | 8.018987670 |
| 6 | 29.936963800 | 7.153431330  | 7.995991670 |
| 6 | 38.550299800 | 6.304133330  | 7.971669670 |
| 6 | 33.529129800 | 21.866299330 | 7.958971670 |
| 6 | 27.462633800 | 7.194260330  | 7.886519670 |
| 6 | 36.084002800 | 6.394915330  | 7.867139670 |
| 6 | 22.441124800 | 22.570133330 | 7.886455670 |
| 6 | 24.901136800 | 22.462167330 | 7.774119670 |
| 6 | 25.000106800 | 7.235992330  | 7.765500670 |
| 6 | 33.624788800 | 6.503376330  | 7.742831670 |
| 6 | 22.530265800 | 7.233665330  | 7.664023670 |
| 6 | 27.382266800 | 22.409969330 | 7.667596670 |
| 6 | 29.855311800 | 22.407709330 | 7.630054670 |
| 6 | 20.064148800 | 7.198594330  | 7.617101670 |
| 6 | 31.172559800 | 6.593206330  | 7.610685670 |
| 6 | 17.601731800 | 7.143120330  | 7.601187670 |
| 6 | 15.154112800 | 7.076477330  | 7.598742670 |

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| 6 | 32.331706800 | 22.424865330 | 7.587856670  |
| 6 | 28.709117800 | 6.633922330  | 7.517368670  |
| 6 | 26.243768800 | 6.686157330  | 7.384891670  |
| 6 | 23.779072800 | 6.684071330  | 7.307802670  |
| 6 | 16.358173800 | 6.498394330  | 7.282057670  |
| 6 | 21.309538800 | 6.639645330  | 7.267807670  |
| 6 | 18.837396800 | 6.576290330  | 7.267817670  |
| 1 | 39.569456800 | 14.698625330 | 11.077025670 |
| 1 | 40.800001800 | 12.601497330 | 10.821218670 |
| 1 | 38.280986800 | 16.773322330 | 10.566228670 |
| 1 | 7.824610800  | 16.564378330 | 10.303378670 |
| 1 | 9.078293800  | 14.445679330 | 10.257916670 |
| 1 | 42.021440800 | 10.556599330 | 10.113911670 |
| 1 | 6.598785800  | 18.699649330 | 9.968302670  |
| 1 | 37.010120800 | 18.700637330 | 9.821301670  |
| 1 | 10.358196800 | 12.374770330 | 9.827139670  |
| 1 | 5.396739800  | 20.802617330 | 9.399084670  |
| 1 | 43.231718800 | 8.566540330  | 9.249639670  |
| 1 | 11.641803800 | 10.395500330 | 9.140962670  |
| 1 | 35.739586800 | 20.537463330 | 8.773907670  |
| 1 | 5.461507800  | 23.177422330 | 8.627489670  |
| 1 | 12.927668800 | 8.460615330  | 8.293077670  |
| 1 | 7.644938800  | 24.324001330 | 8.238234670  |
| 1 | 10.128663800 | 24.247221330 | 8.180500670  |
| 1 | 43.187357800 | 6.317835330  | 8.164616670  |
| 1 | 12.611539800 | 24.107222330 | 8.031016670  |
| 1 | 15.058025800 | 23.904665330 | 7.794172670  |
| 1 | 34.477765800 | 22.312784330 | 7.628410670  |
| 1 | 41.015035800 | 5.245503330  | 7.557743670  |
| 1 | 17.505277800 | 23.675104330 | 7.557350670  |



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| 1 | 38.534314800 | 5.334800330  | 7.451330670  |
| 1 | 14.211190800 | 6.567624330  | 7.352428670  |
| 1 | 36.069965800 | 5.450074330  | 7.304505670  |
| 1 | 33.614166800 | 5.596458330  | 7.121064670  |
| 1 | 19.897970800 | 23.332345330 | 7.158636670  |
| 1 | 24.885993800 | 23.236381330 | 6.994048670  |
| 1 | 32.304490800 | 23.322902330 | 6.954331670  |
| 1 | 29.841714800 | 23.270360330 | 6.948033670  |
| 1 | 22.402987800 | 23.174029330 | 6.969189670  |
| 1 | 27.373937800 | 23.220891330 | 6.925115670  |
| 1 | 31.183380800 | 5.727270330  | 6.933332670  |
| 1 | 28.725549800 | 5.778646330  | 6.827322670  |
| 1 | 16.393734800 | 5.522168330  | 6.777616670  |
| 1 | 18.862772800 | 5.618306330  | 6.728000670  |
| 1 | 21.335571800 | 5.709181330  | 6.682303670  |
| 1 | 26.263455800 | 5.830597330  | 6.694475670  |
| 1 | 23.807613800 | 5.791636330  | 6.665961670  |
| 8 | 24.870083800 | 15.702463330 | 12.397576670 |
| 8 | 28.570332800 | 13.251937330 | 12.763003670 |
| 8 | 32.465402800 | 15.820525330 | 12.712083670 |
| 8 | 36.247152800 | 13.278530330 | 12.622102670 |
| 8 | 17.331649800 | 15.593349330 | 12.535335670 |
| 8 | 21.259913800 | 18.125021330 | 12.406923670 |
| 8 | 21.097709800 | 13.212661330 | 12.393101670 |
| 8 | 28.687200800 | 18.177417330 | 12.205366670 |
| 8 | 13.561968800 | 18.081526330 | 12.167172670 |
| 8 | 32.439608800 | 10.779077330 | 12.129064670 |
| 8 | 24.798310800 | 10.858875330 | 11.861884670 |
| 8 | 17.450560800 | 20.543174330 | 11.606581670 |
| 8 | 25.025520800 | 20.425449330 | 11.299873670 |

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| 8  | 28.611990800 | 8.618277330  | 10.961571670 |
| 8  | 21.286874800 | 22.589534330 | 10.066108670 |
| 8  | 23.632536800 | 16.281852330 | 16.609857670 |
| 8  | 24.154952800 | 18.057067330 | 14.636175670 |
| 8  | 23.110139800 | 14.506701330 | 18.583466670 |
| 8  | 21.015656800 | 16.964071330 | 16.530811670 |
| 58 | 22.808279800 | 18.472773330 | 16.507892670 |
| 58 | 21.840045800 | 14.773261330 | 16.632774670 |
| 8  | 25.803617800 | 13.675401330 | 14.840031670 |
| 8  | 24.078354800 | 18.206148330 | 18.458657670 |
| 8  | 23.186737800 | 14.357621330 | 14.760984670 |
| 58 | 24.979341800 | 15.866257330 | 14.738139670 |
| 8  | 26.771831800 | 17.374847330 | 14.715222670 |
| 8  | 25.727019800 | 13.824482330 | 18.662513670 |
| 8  | 28.866295800 | 14.917412330 | 16.767950670 |
| 8  | 26.249415800 | 15.599632330 | 16.688904670 |
| 58 | 24.902743800 | 16.015338330 | 18.560621670 |
| 58 | 28.042038800 | 17.108334330 | 16.665985670 |
| 58 | 27.073804800 | 13.408822330 | 16.790867670 |
| 8  | 26.695233800 | 17.523928330 | 18.537704670 |

**b) CeO<sub>2</sub>/GP**

|   |              |             |             |
|---|--------------|-------------|-------------|
| 6 | 15.902549760 | 6.419210590 | 7.718457330 |
| 6 | 18.378239760 | 6.422452590 | 7.744584330 |
| 6 | 20.847913760 | 6.420023590 | 7.770210330 |
| 6 | 23.315202760 | 6.417305590 | 7.790701330 |
| 6 | 25.780053760 | 6.415997590 | 7.803061330 |
| 6 | 28.244171760 | 6.415360590 | 7.809359330 |
| 6 | 30.708794760 | 6.416738590 | 7.818309330 |
| 6 | 33.173147760 | 6.420133590 | 7.833193330 |
| 6 | 35.637009760 | 6.423723590 | 7.850210330 |

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| 6 | 40.577686760 | 6.427547590  | 7.890948330 |
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