

**Supporting Information:**

**Supplemental Information: A Systematic Search  
for the Adsorption Motif of All Stereoisomers of  
Propylene Glycol on a Palladium(111) Surface for  
Fuel Cell Applications**

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Fullerton, CA, 92831, USA*

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**Molecular Positions for the most favourable systems**

12PGS\_Flat

Absolute Energy: -304.29042770504816 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197774, 0.0, 6.000000000000001]

Pd [8.18617520579666, 0.0, 6.000000000000001]

Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]

Pd [4.09308760289833, 2.3631452293500708, 6.0000000000000001]  
Pd [6.821812671497217, 2.3631452293500708, 6.0000000000000001]  
Pd [9.550537740096104, 2.3631452293500708, 6.0000000000000001]  
Pd [0.0, 4.7262904587001415, 6.0000000000000001]  
Pd [2.728725068598887, 4.7262904587001415, 6.0000000000000001]  
Pd [5.457450137197774, 4.7262904587001415, 6.0000000000000001]  
Pd [8.186175205796666, 4.7262904587001415, 6.0000000000000001]  
Pd [1.3643625342994434, 7.089435688050212, 6.0000000000000001]  
Pd [4.09308760289833, 7.089435688050212, 6.0000000000000001]  
Pd [6.821812671497217, 7.089435688050212, 6.0000000000000001]  
Pd [9.550537740096104, 7.089435688050212, 6.0000000000000001]  
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Pd [6.808910577295129, 0.8276679354849412, 8.327239049988643]  
Pd [9.537163682946659, 0.8280927729140967, 8.32699086278343]  
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Pd [5.448007764256732, 3.193754933273248, 8.329003333620857]  
Pd [8.173085748117975, 3.1928870829576317, 8.334694568330743]  
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Pd [6.81138609476896, 5.554265634310797, 8.338404737776873]  
Pd [9.534901269285374, 5.555992604000302, 8.334668636973237]  
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O [9.44958602558155, 2.7949122182347557, 16.177439766456445]  
H [9.727361160517866, 2.419841890935031, 15.304401345698066]

12PGS-sOHd

Absolute Energy: -304.2476817328358 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197774, 0.0, 6.000000000000001]

Pd [8.18617520579666, 0.0, 6.000000000000001]

Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]  
Pd [4.09308760289833, 2.3631452293500708, 6.000000000000001]  
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H [5.870797021595938, 2.9011646022802022, 15.469255943026749]

12PGR\_Flat

Absolute Energy: -304.28617459020916 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197774, 0.0, 6.000000000000001]

Pd [8.18617520579666, 0.0, 6.000000000000001]  
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H [6.428288993488665, 2.5788556177398716, 15.282307789109003]

12PGR-sOHd

Absolute Energy: -304.23943464218024 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197774, 0.0, 6.000000000000001]  
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Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]  
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Pd [9.550537740096104, 2.3631452293500708, 6.000000000000001]  
Pd [0.0, 4.7262904587001415, 6.000000000000001]  
Pd [2.728725068598887, 4.7262904587001415, 6.000000000000001]  
Pd [5.457450137197774, 4.7262904587001415, 6.000000000000001]  
Pd [8.18617520579666, 4.7262904587001415, 6.000000000000001]  
Pd [1.3643625342994434, 7.089435688050212, 6.000000000000001]  
Pd [4.09308760289833, 7.089435688050212, 6.000000000000001]  
Pd [6.821812671497217, 7.089435688050212, 6.000000000000001]  
Pd [9.550537740096104, 7.089435688050212, 6.000000000000001]  
Pd [1.3528551589414424, 0.8300292340276173, 8.328105421243349]  
Pd [4.081205874034844, 0.8279355184946863, 8.327540778722007]  
Pd [6.810489876072768, 0.8193343819122625, 8.337795789295667]  
Pd [9.53907408896175, 0.8285731874892516, 8.326775022454145]  
Pd [-0.011206277192935979, 3.1933324623801975, 8.327485432727116]  
Pd [2.7173988133357234, 3.1931690562093538, 8.328296937719731]  
Pd [5.446014416727228, 3.1882659145811503, 8.328172592625243]  
Pd [8.173893884915818, 3.1885420484833, 8.328864282639207]  
Pd [1.3531929292014215, 5.556803659725043, 8.32766861939884]  
Pd [4.0830599626343655, 5.555616674223789, 8.328673070622456]  
Pd [6.808863502157312, 5.552824907509784, 8.333718832850849]  
Pd [9.53725513519438, 5.5556450275012885, 8.327028001266816]  
Pd [-0.012411730603584388, 7.919050807152708, 8.327057193497318]

Pd [2.716922442597199, 7.9188538626127984, 8.327390140139045]  
Pd [5.44779376869874, 7.915218583317051, 8.339398994653294]  
Pd [8.170016544880246, 7.916506653411567, 8.338823203907305]  
Pd [-0.04331737018900187, 1.6688317957339012, 10.632803136380797]  
Pd [2.685541889766147, 1.6701094105401766, 10.632518391167757]  
Pd [5.41579569235208, 1.6592150693582108, 10.631810804646205]  
Pd [8.141482973167175, 1.6555980473140512, 10.633329756633666]  
Pd [1.3213555834555957, 4.03295750121528, 10.633659585067713]  
Pd [4.051392677879472, 4.031968452496681, 10.63157285752098]  
Pd [6.778808469144654, 4.021478594873575, 10.632374329386867]  
Pd [9.506482641943538, 4.028925672773414, 10.629017486698123]  
Pd [-0.0439053891020735, 6.393994060027458, 10.630548834192574]  
Pd [2.6873909680082897, 6.395312301857689, 10.633051344800869]  
Pd [5.421369725769923, 6.392340344866145, 10.655770220070174]  
Pd [8.139886744966603, 6.38994298217109, 10.6467017926207]  
Pd [1.3204429251346703, 8.758253032027213, 10.632395177611642]  
Pd [4.046370076184309, 8.757147400387675, 10.632269238289965]  
Pd [6.770571034050208, 8.72429992840992, 10.68932893509372]  
Pd [9.507475196954132, 8.75699962728239, 10.631876352309797]  
Pd [-0.08347631880747097, 0.165366762007032, 12.953518716065364]  
Pd [2.6437689804867, 0.16635923296073157, 12.952076168660536]  
Pd [5.3691710558934505, 0.17194174208529484, 12.954272816388482]  
Pd [8.10600996960428, 0.17181594756061286, 12.956560034471059]  
Pd [1.2800365522885255, 2.5276524973494654, 12.951664063313943]  
Pd [4.008383946864428, 2.527808761119572, 12.951099342636487]  
Pd [6.737342833137933, 2.5265658248806955, 12.95354319476793]  
Pd [9.467304697666288, 2.528278575988474, 12.95210549207433]

Pd [-0.0841186303081659, 4.890744075422162, 12.9529829394345]  
Pd [2.6444127661054466, 4.890467689178996, 12.951204555827157]  
Pd [5.371066690379796, 4.883859644883998, 12.949992638843616]  
Pd [8.10585256191312, 4.881543607070007, 12.946229848381547]  
Pd [1.2797027249091346, 7.254890325620245, 12.953427668518186]  
Pd [4.004690877119546, 7.255399545285203, 12.951491495383523]  
Pd [6.7351663748877035, 7.2538922532031656, 13.09754637649459]  
Pd [9.47188723694162, 7.249331288813515, 12.945002217034943]  
O [9.18296956776713, 7.584568087914539, 16.164561393991406]  
C [8.216538399917292, 8.65839280903884, 16.19013060492086]  
C [6.829340038267585, 8.017489133363624, 16.272979717139858]  
C [8.486392712596365, 9.589836908671215, 17.356836742294426]  
H [8.281148640208905, 9.221737668813105, 15.2270570777615]  
H [6.039127232284789, 8.726277613795396, 15.994062203708701]  
H [6.642268623646183, 7.641839382176026, 17.294204573242137]  
H [9.682129136264617, 7.638583351554402, 15.311257032451321]  
H [8.50443608524747, 9.019549937338311, 18.297035863845156]  
H [9.454782468870539, 10.091383529741574, 17.238020123602976]  
H [7.704951504726813, 10.359991596693616, 17.431725011346476]  
O [6.73377507381688, 6.8923944111834885, 15.372031855154239]  
H [7.618573967620464, 6.4536225868018455, 15.469207240130663]

13PG\_OHside\_2ndFavourable

Absolute Energy: -304.2554840046908 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]  
Pd [5.457450137197774, 0.0, 6.000000000000001]  
Pd [8.18617520579666, 0.0, 6.000000000000001]  
Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]  
Pd [4.09308760289833, 2.3631452293500708, 6.000000000000001]  
Pd [6.821812671497217, 2.3631452293500708, 6.000000000000001]  
Pd [9.550537740096104, 2.3631452293500708, 6.000000000000001]  
Pd [0.0, 4.7262904587001415, 6.000000000000001]  
Pd [2.728725068598887, 4.7262904587001415, 6.000000000000001]  
Pd [5.457450137197774, 4.7262904587001415, 6.000000000000001]  
Pd [8.18617520579666, 4.7262904587001415, 6.000000000000001]  
Pd [1.3643625342994434, 7.089435688050212, 6.000000000000001]  
Pd [4.09308760289833, 7.089435688050212, 6.000000000000001]  
Pd [6.821812671497217, 7.089435688050212, 6.000000000000001]  
Pd [9.550537740096104, 7.089435688050212, 6.000000000000001]  
Pd [1.3626528373927569, 0.8235344824267065, 8.325539343578757]  
Pd [4.09081177821588, 0.819627406042714, 8.32407620580839]  
Pd [6.818550493469686, 0.8204958684748697, 8.325153120318493]  
Pd [9.547955797280812, 0.8241545124149842, 8.324541817236106]  
Pd [-0.0017459279949857505, 3.187343665301473, 8.324633579831161]  
Pd [2.729406737389301, 3.1851666361546744, 8.329120012125697]  
Pd [5.452532023777045, 3.183310719948663, 8.333742382566918]  
Pd [8.18088144725717, 3.185677019142614, 8.324975995808154]  
Pd [1.3618855547343187, 5.548607289406178, 8.324702320802416]  
Pd [4.091992155318346, 5.541536598482452, 8.334131664309451]  
Pd [6.816364049443604, 5.544861734588744, 8.332567208992717]  
Pd [9.547247611361929, 5.549358041684611, 8.323906244503286]

Pd [-0.00262474673972237, 7.912995942223028, 8.324998329180362]  
Pd [2.726473230325157, 7.910122398236744, 8.324255584773]  
Pd [5.4547863957158675, 7.905206845542426, 8.328085360500978]  
Pd [8.18267922317529, 7.911718636476135, 8.32371388092675]  
Pd [-0.019272962056249256, 1.6137633305906565, 10.621847091468032]  
Pd [2.7109989457404726, 1.6156842989271745, 10.62021070105033]  
Pd [5.436405335888656, 1.6128028978763531, 10.62021272778264]  
Pd [8.165168188860804, 1.614868894796443, 10.618927328538428]  
Pd [1.3461779904840838, 3.9765232977662155, 10.620985651615547]  
Pd [4.078307619985052, 3.987112355078032, 10.664672777009665]  
Pd [6.792948327611999, 3.9812032096425987, 10.6384647135764]  
Pd [9.529137524587455, 3.9759009491069586, 10.618626707857782]  
Pd [-0.020939845166528245, 6.339058819082986, 10.620412496548429]  
Pd [2.704860103917346, 6.341182439680767, 10.620008669686362]  
Pd [5.432419651208967, 6.3361724176028815, 10.64539402255007]  
Pd [8.166495759959284, 6.34074714608341, 10.620046127310765]  
Pd [1.3436959235157173, 8.703568847925142, 10.620684482128448]  
Pd [4.07283131485796, 8.702261031781154, 10.617782084429173]  
Pd [6.801665233528159, 8.700779685673025, 10.618924581681464]  
Pd [9.530587771295986, 8.703432464312147, 10.620621275280458]  
Pd [-0.08210109272559821, 0.022922885110325947, 12.947603413023764]  
Pd [2.645725732871371, 0.023558217531106044, 12.946605391567923]  
Pd [5.3745381119161975, 0.023351415266462547, 12.946823035109695]  
Pd [8.106544414731253, 0.022158637685874335, 12.948048869757319]  
Pd [1.2821494108031617, 2.386233182837029, 12.94730326336394]  
Pd [4.008297200910741, 2.3776894059368905, 12.947647785961355]  
Pd [6.747012757553929, 2.370639915328964, 12.943164785747376]

Pd [9.47042119996258, 2.3849791941268754, 12.948542461938457]  
Pd [-0.0821394133193554, 4.750898117213754, 12.949550350734068]  
Pd [2.642006908527416, 4.751896472494284, 12.949503802000194]  
Pd [5.383533732786684, 4.739731706577408, 13.052870677884263]  
Pd [8.11470444879009, 4.745579343111133, 12.939374270490392]  
Pd [1.281427296412209, 7.114580239467902, 12.948392472908786]  
Pd [4.005783746251804, 7.1191948930522315, 12.942914969821793]  
Pd [6.743221371114232, 7.118503360300838, 12.94612576682777]  
Pd [9.469793721687852, 7.114575035416503, 12.9517522708721]  
C [5.106044194500726, 5.668845232567002, 16.190467167707574]  
C [6.087170523626962, 6.828942729629327, 16.133373211534185]  
C [7.486686926239607, 6.496109048175918, 16.64395410399267]  
H [6.1479590255676655, 7.188813845470833, 15.076417198589851]  
H [5.686032915756997, 7.678334364604326, 16.710083860104127]  
O [5.509150885946583, 4.565600733765797, 15.334052430404721]  
H [6.488569041494331, 4.475828754817845, 15.511049125476797]  
O [8.007712183006923, 5.254660136108205, 16.105749363598708]  
H [8.45340126560528, 5.447267062206925, 15.240699805800988]  
H [4.104854780829161, 5.9721774483456125, 15.855822375234817]  
H [5.023899626465543, 5.271424605054388, 17.218061130529634]  
H [8.178927040015429, 7.323389253954802, 16.423280545593702]  
H [7.470267011613043, 6.348286782095042, 17.7344992262556]

13PG\_OHside\_mostFavourable

Absolute Energy: -304.36428121850116 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]



Pd [0.0, 0.0, 6.000000000000001]  
Pd [2.728725068598887, 0.0, 6.000000000000001]  
Pd [5.457450137197774, 0.0, 6.000000000000001]  
Pd [8.18617520579666, 0.0, 6.000000000000001]  
Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]  
Pd [4.09308760289833, 2.3631452293500708, 6.000000000000001]  
Pd [6.821812671497217, 2.3631452293500708, 6.000000000000001]  
Pd [9.550537740096104, 2.3631452293500708, 6.000000000000001]  
Pd [0.0, 4.7262904587001415, 6.000000000000001]  
Pd [2.728725068598887, 4.7262904587001415, 6.000000000000001]  
Pd [5.457450137197774, 4.7262904587001415, 6.000000000000001]  
Pd [8.18617520579666, 4.7262904587001415, 6.000000000000001]  
Pd [1.3643625342994434, 7.089435688050212, 6.000000000000001]  
Pd [4.09308760289833, 7.089435688050212, 6.000000000000001]  
Pd [6.821812671497217, 7.089435688050212, 6.000000000000001]  
Pd [9.550537740096104, 7.089435688050212, 6.000000000000001]  
Pd [1.3517631009355864, 0.8307213629139366, 8.326150226716374]  
Pd [4.081229525860973, 0.8287545362525401, 8.327276967149121]  
Pd [6.808889149350098, 0.8252745660668006, 8.331432397663425]  
Pd [9.537741053659294, 0.8294779539540921, 8.326770788777992]  
Pd [-0.012996508016115847, 3.193850389287608, 8.327275051668419]  
Pd [2.7163700602079923, 3.193158424855266, 8.32582353398362]  
Pd [5.445586595027561, 3.1905649802342166, 8.326926738968584]  
Pd [8.173415618889992, 3.1912859737532084, 8.326747263870285]  
Pd [1.352471905989794, 5.55712343286318, 8.327258856125722]  
Pd [4.081907921767653, 5.556191961769036, 8.327510113218809]  
Pd [6.809037315393991, 5.554723051636007, 8.331271497153088]

Pd [9.537051787636278, 5.556465582508074, 8.326228844621697]  
Pd [-0.013080071642331784, 7.919908990294507, 8.32659375514986]  
Pd [2.7169085613249178, 7.91893729601115, 8.327197956462392]  
Pd [5.446277791474622, 7.916803543875108, 8.334889530444121]  
Pd [8.172109071208352, 7.9175715885885225, 8.331960206362677]  
Pd [-0.04389670535031609, 1.669636861732451, 10.631203991899033]  
Pd [2.6850301961296807, 1.669589082818327, 10.630134277095843]  
Pd [5.413958276324608, 1.663225576510399, 10.629796596264391]  
Pd [8.14165842575805, 1.6658397978616781, 10.629629648714417]  
Pd [1.3202432470255165, 4.032787189100849, 10.629900778877433]  
Pd [4.048876059067596, 4.031729161265412, 10.626411657691856]  
Pd [6.778195532497265, 4.028661771314371, 10.629285195850315]  
Pd [9.50646291954751, 4.032273174155618, 10.630240169691493]  
Pd [-0.043270299915599775, 6.394489754978563, 10.629576238210342]  
Pd [2.6889305085629327, 6.397066457171305, 10.636015683993092]  
Pd [5.419503136094284, 6.397782084465605, 10.647203749522363]  
Pd [8.142459165875096, 6.395622550932229, 10.641870075594623]  
Pd [1.3204741707888117, 8.759315371573544, 10.63101520512595]  
Pd [4.048100481381108, 8.755503041344962, 10.633077532964224]  
Pd [6.780483133841582, 8.743609374910996, 10.654486731833508]  
Pd [9.50849321309622, 8.758630137992318, 10.632074593524091]  
Pd [-0.08239380555895773, 0.16775211971354603, 12.951940449607381]  
Pd [2.64248124707939, 0.1702267007491698, 12.950848028294539]  
Pd [5.374674480165356, 0.1739346056730522, 12.94588651551304]  
Pd [8.107591798889798, 0.17494867001949113, 12.951537776951985]  
Pd [1.2801845389136801, 2.5282629592406574, 12.950969533510367]  
Pd [4.0080291060223585, 2.528781355849115, 12.951270762151559]

Pd [6.73866313149142, 2.5278935109183083, 12.95142069162253]  
Pd [9.467694579760835, 2.528170493228163, 12.950089433163168]  
Pd [-0.08226159221059459, 4.890140256065519, 12.951293858061016]  
Pd [2.6433151823931333, 4.885521690632866, 12.949845437771124]  
Pd [5.370998565807056, 4.878224792271121, 12.941338698517477]  
Pd [8.106263584902281, 4.8807403428732865, 12.947942572783335]  
Pd [1.2784435649692976, 7.255343908477892, 12.952013939423543]  
Pd [4.010177230518831, 7.256483113201341, 12.955803216159426]  
Pd [6.776123236944794, 7.2489052065374855, 13.024795386595473]  
Pd [9.478613287328653, 7.256245929158435, 12.951032948216767]  
C [4.104673776374571, 8.25824519557373, 16.328338684374277]  
C [5.477364954048618, 8.872840837495987, 16.116974327643906]  
C [6.661190619614991, 7.937969845998401, 16.31963268511302]  
H [5.534868108159147, 9.306965858897826, 15.088167890992615]  
H [5.57999816399561, 9.727013389394711, 16.804756223270385]  
O [3.99866496617535, 7.050916579068327, 15.524111215612116]  
H [3.068135838031194, 6.743005300652023, 15.513293352497849]  
O [6.731001934865871, 6.854308472890827, 15.359406249011888]  
H [5.848815761301488, 6.413071845625466, 15.372537497873141]  
H [3.322960541603579, 8.97395023053893, 16.02865959855105]  
H [3.955016896398517, 7.984753383511109, 17.387393133116436]  
H [7.6034605362305845, 8.489429551593615, 16.204273676590507]  
H [6.639834285693905, 7.49223115076013, 17.33047763341718]

12PG\_gas

Absolute Energy: -70.29193609131168 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]  
O [8.106594953323377, 5.160753397783514, 15.335643589612582]  
C [7.561831747222204, 4.28859478802137, 16.337573146792]  
C [6.048910470264612, 4.4050821689022035, 16.289512990987756]  
C [8.03730703703184, 2.8609639223943937, 16.102722980842948]  
H [7.927206752181147, 4.60516018880527, 17.335729953104437]  
H [5.58353239333197, 3.789553647508321, 17.071794853241308]  
H [5.6657449658691075, 4.083027518078731, 15.310538473747647]  
H [9.052027896529733, 4.913385182856004, 15.26054228835339]  
H [7.6619139642916885, 2.5034105842397425, 15.127586858608389]  
H [7.653530319559991, 2.199791317775162, 16.900346480404114]  
H [5.746930102210485, 5.447701851071608, 16.448150113658848]  
O [9.477166384787651, 2.8965733964147904, 16.1118644566694]  
H [9.809303816469615, 2.04606679291804, 15.771223256939413]

### 13PG\_gas

Absolute Energy: -70.29193609131168 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]  
O [8.106594953323377, 5.160753397783514, 15.335643589612582]  
C [7.561831747222204, 4.28859478802137, 16.337573146792]  
C [6.048910470264612, 4.4050821689022035, 16.289512990987756]  
C [8.03730703703184, 2.8609639223943937, 16.102722980842948]  
H [7.927206752181147, 4.60516018880527, 17.335729953104437]  
H [5.58353239333197, 3.789553647508321, 17.071794853241308]  
H [5.6657449658691075, 4.083027518078731, 15.310538473747647]  
H [9.052027896529733, 4.913385182856004, 15.26054228835339]

H [7.6619139642916885, 2.5034105842397425, 15.127586858608389]  
H [7.653530319559991, 2.199791317775162, 16.900346480404114]  
H [5.746930102210485, 5.447701851071608, 16.448150113658848]  
O [9.477166384787651, 2.8965733964147904, 16.11186445666694]  
H [9.809303816469615, 2.04606679291804, 15.771223256939413]

Garcia\_12PG

Absolute Energy: -304.2129106487208 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197775, 0.0, 6.000000000000001]

Pd [8.18617520579666, 0.0, 6.000000000000001]

Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]

Pd [4.093087602898331, 2.3631452293500708, 6.000000000000001]

Pd [6.821812671497218, 2.3631452293500708, 6.000000000000001]

Pd [9.550537740096106, 2.3631452293500708, 6.000000000000001]

Pd [0.0, 4.7262904587001415, 6.000000000000001]

Pd [2.728725068598887, 4.7262904587001415, 6.000000000000001]

Pd [5.457450137197775, 4.7262904587001415, 6.000000000000001]

Pd [8.18617520579666, 4.7262904587001415, 6.000000000000001]

Pd [1.3643625342994434, 7.089435688050212, 6.000000000000001]

Pd [4.09308760289833, 7.089435688050212, 6.000000000000001]

Pd [6.821812671497218, 7.089435688050212, 6.000000000000001]

Pd [9.550537740096106, 7.089435688050212, 6.000000000000001]

Pd [1.352099691522154, 0.8294380322559618, 8.327518415401716]

Pd [4.08163892291256, 0.8256685680175542, 8.327367679846533]  
Pd [6.809195013022107, 0.8255313777465225, 8.328424812998911]  
Pd [9.537768415409333, 0.8295018092007864, 8.327557051089105]  
Pd [-0.012510668737024435, 3.1930438596231823, 8.327344948084878]  
Pd [2.7184966008313687, 3.192396683239997, 8.327805300822863]  
Pd [5.444881671585148, 3.1900165101865743, 8.333902458401175]  
Pd [8.171495555491413, 3.1923825311313037, 8.327619961025635]  
Pd [1.3521574957693605, 5.555231906834548, 8.327171071633074]  
Pd [4.082886483544742, 5.552682112893792, 8.337097583026488]  
Pd [6.805814088285333, 5.553360611387335, 8.336431672162602]  
Pd [9.537397915016875, 5.5551436246937795, 8.326995016961423]  
Pd [-0.012448435603737781, 7.918609112417791, 8.327560411515853]  
Pd [2.7165676695609595, 7.917247734541575, 8.326715233158572]  
Pd [5.445884940803369, 7.909330943269155, 8.336567739496646]  
Pd [8.174187240694193, 7.91702519338857, 8.32678169186625]  
Pd [-0.042942017972618936, 1.6681291875025093, 10.63286092721474]  
Pd [2.6866320258438803, 1.6676115592048202, 10.628902016509267]  
Pd [5.414921029560504, 1.6610125608740776, 10.63166538285247]  
Pd [8.142261896982887, 1.667345355518615, 10.63034515133745]  
Pd [1.3224198191817473, 4.029609005686232, 10.631308342984072]  
Pd [4.056011358595585, 4.031027723502531, 10.650981602304318]  
Pd [6.776606836745709, 4.030268917586282, 10.648378182392399]  
Pd [9.50612060054734, 4.030721690105413, 10.631428053943312]  
Pd [-0.043112737639271516, 6.393617191144362, 10.632403976257118]  
Pd [2.683049235720674, 6.393755901211513, 10.631433434354832]  
Pd [5.407853147267254, 6.365148624442631, 10.684499031222796]  
Pd [8.142652080278964, 6.394041577617507, 10.63112311456769]

Pd [1.321553534224466, 8.757669598724084, 10.63222784830601]  
Pd [4.051398438823671, 8.749480768596927, 10.631080362580256]  
Pd [6.7772676838396855, 8.748221472305843, 10.631834279077951]  
Pd [9.507270433970731, 8.757731079030382, 10.631846496360904]  
Pd [-0.08373447018071017, 0.16555293269752014, 12.95099348570007]  
Pd [2.644719769169316, 0.16618827054130586, 12.95221802014331]  
Pd [5.3726866303489595, 0.16391875895066654, 12.954861406207526]  
Pd [8.102394619561593, 0.16498754574725652, 12.951301693061035]  
Pd [1.28071010895666542, 2.5275169866950082, 12.952515066870504]  
Pd [4.005159474219498, 2.521919991092357, 12.94515150349224]  
Pd [6.739184248123444, 2.5203114779625815, 12.947258662445996]  
Pd [9.467210466021971, 2.5282402447220096, 12.951727099973413]  
Pd [-0.08364029520577931, 4.891835216891054, 12.95127469682429]  
Pd [2.6392287973250177, 4.893221080087154, 12.948424522978453]  
Pd [5.372654709498962, 4.910161013421495, 13.084149837712777]  
Pd [8.108131040995811, 4.896258962280247, 12.949209476130754]  
Pd [1.279841173460951, 7.256942565328455, 12.950994184064164]  
Pd [4.004747104024893, 7.264644106915008, 12.954196366733072]  
Pd [6.742018404590447, 7.264443162913202, 12.954340301330964]  
Pd [9.467450962648545, 7.257324651090831, 12.951148145420424]  
C [5.3247089864343815, 2.6362482684627033, 16.84486141567653]  
H [4.220136206575603, 1.7164829578516476, 15.469032176307566]  
H [4.36385720415164, 4.1343570371243565, 15.41819847145559]  
H [5.900599306216172, 1.730338602890415, 17.0948153845832]  
C [6.147761375743898, 3.5421562718401796, 15.929399920083256]  
H [5.073563854582793, 3.1632727023592335, 17.778771759138856]  
O [4.064226688365271, 2.315756833263545, 16.23900480142962]

H [6.508212324458347, 2.9105861924016914, 15.070442329826564]  
C [7.337065460704424, 4.214267913124734, 16.574245959298942]  
H [7.01929245727934, 4.858243572379493, 17.406539270750972]  
H [8.045497383169758, 3.4630653728051977, 16.95003199561417]  
O [5.25983057476911, 4.561521970706357, 15.394994931708787]  
H [7.866159461695419, 4.832642697683616, 15.833034162164298]

### Garcia\_13PG

Absolute Energy: -304.254104246982 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197774, 0.0, 6.000000000000001]

Pd [8.18617520579666, 0.0, 6.000000000000001]

Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]

Pd [4.09308760289833, 2.3631452293500708, 6.000000000000001]

Pd [6.821812671497217, 2.3631452293500708, 6.000000000000001]

Pd [9.550537740096104, 2.3631452293500708, 6.000000000000001]

Pd [0.0, 4.7262904587001415, 6.000000000000001]

Pd [2.728725068598887, 4.7262904587001415, 6.000000000000001]

Pd [5.457450137197774, 4.7262904587001415, 6.000000000000001]

Pd [8.18617520579666, 4.7262904587001415, 6.000000000000001]

Pd [1.3643625342994434, 7.089435688050212, 6.000000000000001]

Pd [4.09308760289833, 7.089435688050212, 6.000000000000001]

Pd [6.821812671497217, 7.089435688050212, 6.000000000000001]

Pd [9.550537740096104, 7.089435688050212, 6.000000000000001]



Pd [1.3621651822236982, 0.822593081222905, 8.326458321886042]  
Pd [4.090582690905889, 0.8191855185406846, 8.325353576378784]  
Pd [6.818376139603822, 0.82042595941106, 8.32484166826374]  
Pd [9.54746077948409, 0.8231118080770446, 8.326244471526948]  
Pd [-0.0024767811590442434, 3.1863897579509133, 8.324966979299202]  
Pd [2.7285744085951427, 3.184109746360842, 8.32885519528581]  
Pd [5.452959249944715, 3.1832197632444967, 8.335138133430197]  
Pd [8.180797550110931, 3.1853646001431652, 8.325382705790735]  
Pd [1.3616097544359294, 5.54792108726308, 8.324960532249245]  
Pd [4.091686485704632, 5.541264113548944, 8.334099277951836]  
Pd [6.81668258102863, 5.5444933545458825, 8.33215133222663]  
Pd [9.547414736840258, 5.548651548633493, 8.32499903837556]  
Pd [-0.0028432640107762717, 7.912209921190962, 8.32577363649811]  
Pd [2.7267199122268377, 7.90934965723263, 8.325153730275288]  
Pd [5.454272097276772, 7.9048671923148826, 8.328565774419117]  
Pd [8.183055535883456, 7.910783896227901, 8.324975583992714]  
Pd [-0.019305863813288936, 1.613868711327673, 10.622444324154728]  
Pd [2.711333436427574, 1.6154487601516967, 10.620923415777348]  
Pd [5.4372057947138535, 1.613149431846083, 10.621389529873868]  
Pd [8.165107480205341, 1.6150831565242934, 10.620450249654228]  
Pd [1.3454560568013498, 3.97651875728224, 10.62052968261548]  
Pd [4.076820846762952, 3.9853875802835095, 10.66076569860301]  
Pd [6.795222121484693, 3.981867327909517, 10.640249116961357]  
Pd [9.529927020647136, 3.9754607604153662, 10.61876330274553]  
Pd [-0.020310920564005203, 6.339195901589767, 10.621287368801218]  
Pd [2.70551017770156, 6.341765010688288, 10.622097495767516]  
Pd [5.432982106932811, 6.334796263964813, 10.642763582837047]

Pd [8.167284744735314, 6.340069448584509, 10.62036202992853]  
Pd [1.344190528305001, 8.703984622185825, 10.621854167615547]  
Pd [4.07367160339597, 8.701933928987147, 10.61962827641434]  
Pd [6.802305062756016, 8.702252164330094, 10.61855210680448]  
Pd [9.530802865709717, 8.703580741723387, 10.621616775589944]  
Pd [-0.0819314907262, 0.023399053026037155, 12.948339877988742]  
Pd [2.646157035809105, 0.023979035754908406, 12.947594540710806]  
Pd [5.376250410895094, 0.022192821354725226, 12.949181652714062]  
Pd [8.105451259603583, 0.020949273555457438, 12.94963486903948]  
Pd [1.2827047370341131, 2.386404207614285, 12.948015738935995]  
Pd [4.008590763753812, 2.378170949036466, 12.948115324293058]  
Pd [6.746963288003541, 2.3710783635146098, 12.945327610584288]  
Pd [9.470507313738421, 2.3839399504173806, 12.94748842239008]  
Pd [-0.08081451978149025, 4.750964669272073, 12.947675328273478]  
Pd [2.6426863069617155, 4.751343124426865, 12.948032798850159]  
Pd [5.394630872866516, 4.741525263790065, 13.036535940963402]  
Pd [8.119016330101585, 4.746506308444483, 12.941648733304898]  
Pd [1.2821450802075423, 7.115242772913925, 12.948492280008551]  
Pd [4.0099465599624455, 7.119205209712303, 12.947669356396126]  
Pd [6.743627814349135, 7.122394284916016, 12.94437828668582]  
Pd [9.46963624292793, 7.115404928456629, 12.949911653500212]  
C [4.599049334624976, 5.220437731252661, 16.16277516949156]  
C [4.851250562692855, 6.718653926799798, 16.232394080999782]  
C [6.233355846822779, 7.08809364119184, 16.771513069095633]  
H [4.713332182433592, 7.156982658828076, 15.217533641073317]  
H [4.084600723105181, 7.183030301947082, 16.87399801988037]  
O [5.5513514696856525, 4.541787474553408, 15.298582832475114]

H [6.425699295611081, 4.9878229016520415, 15.499475986662615]  
O [7.31349026343804, 6.405639751781601, 16.085829809397488]  
H [7.493026711876561, 6.875179169402969, 15.228759814764208]  
H [3.601239552007205, 5.000841733038627, 15.759038971104115]  
H [4.678675115464889, 4.759346770031571, 17.163354855047647]  
H [6.390022546862588, 8.176216254485793, 16.72648323093162]  
H [6.328807035880783, 6.7777357465928265, 17.82376686461355]

#### Pd111\_slab

Absolute Energy: -233.02761885302021 eV

Cell: [10.914900274395547, 9.452580917400283, 27.808]

Pd [0.0, 0.0, 6.000000000000001]

Pd [2.728725068598887, 0.0, 6.000000000000001]

Pd [5.457450137197774, 0.0, 6.000000000000001]

Pd [8.18617520579666, 0.0, 6.000000000000001]

Pd [1.3643625342994434, 2.3631452293500708, 6.000000000000001]

Pd [4.09308760289833, 2.3631452293500708, 6.000000000000001]

Pd [6.821812671497217, 2.3631452293500708, 6.000000000000001]

Pd [9.550537740096104, 2.3631452293500708, 6.000000000000001]

Pd [0.0, 4.7262904587001415, 6.000000000000001]

Pd [2.728725068598887, 4.7262904587001415, 6.000000000000001]

Pd [5.457450137197774, 4.7262904587001415, 6.000000000000001]

Pd [8.18617520579666, 4.7262904587001415, 6.000000000000001]

Pd [1.3643625342994434, 7.089435688050212, 6.000000000000001]

Pd [4.09308760289833, 7.089435688050212, 6.000000000000001]

Pd [6.821812671497217, 7.089435688050212, 6.000000000000001]

Pd [9.550537740096104, 7.089435688050212, 6.000000000000001]  
Pd [1.3520588217247613, 0.830097411681692, 8.327648419163332]  
Pd [4.08135377933042, 0.8298387321593931, 8.328263454184324]  
Pd [6.8103260731561495, 0.8289120587744822, 8.329625850306307]  
Pd [9.538385972489536, 0.8289146617553338, 8.329939754619797]  
Pd [-0.012169498174880765, 3.1922640051341933, 8.329342754238324]  
Pd [2.7166576950240553, 3.1931522131943852, 8.328336093297922]  
Pd [5.4452231976190895, 3.1922679824346356, 8.3291289378431]  
Pd [8.173950521901387, 3.1917173127865075, 8.329883282666062]  
Pd [1.3520540606782914, 5.556178050267715, 8.328164936601139]  
Pd [4.080664462531072, 5.555994196453262, 8.328408652827918]  
Pd [6.809158793556779, 5.555471862489543, 8.328382145154563]  
Pd [9.538398371286506, 5.554578443229337, 8.329495416571246]  
Pd [-0.012469951134148649, 7.9185399180923, 8.328453961186629]  
Pd [2.716377068595544, 7.9197336233491455, 8.327600173706633]  
Pd [5.445279777464255, 7.918937655838625, 8.32856682650911]  
Pd [8.174036310236302, 7.918138917414886, 8.328898216550016]  
Pd [-0.042442957604996515, 1.670386610619342, 10.634545458309608]  
Pd [2.6857736774462726, 1.6730117413733154, 10.632855271439459]  
Pd [5.415393295028251, 1.670352204522753, 10.634600230489603]  
Pd [8.143862177825994, 1.6681656919733592, 10.636299001800145]  
Pd [1.3221318759990093, 4.035655711290009, 10.633662976755385]  
Pd [4.050573361089536, 4.035042773566235, 10.633964170926467]  
Pd [6.779396268654743, 4.032843141143927, 10.634584311019559]  
Pd [9.50873930045707, 4.031290154187833, 10.636115192706345]  
Pd [-0.042671924825083384, 6.39620483758906, 10.633849466094471]  
Pd [2.68561039473102, 6.399313267605914, 10.632905382503118]

Pd [5.4144810287419585, 6.396600701245596, 10.633269128909914]  
Pd [8.14376441277268, 6.392851086471316, 10.634374333899906]  
Pd [1.3207817146151446, 8.761845383330028, 10.632378221527599]  
Pd [4.050164481916921, 8.761257102643638, 10.633372577838337]  
Pd [6.779578205393339, 8.75721957460413, 10.634501229942488]  
Pd [9.507770726165742, 8.757305861506554, 10.634629894078259]  
Pd [-0.08356165958774148, 0.16566662379533315, 12.951705671677]  
Pd [2.6445732931292523, 0.16723783922295388, 12.950529753654953]  
Pd [5.3731602271408905, 0.16655063465966408, 12.951406286067817]  
Pd [8.101938480257173, 0.16505084194762934, 12.952312925839271]  
Pd [1.2811876887054752, 2.529589860383159, 12.951507942009787]  
Pd [4.0085182396580485, 2.530359355460863, 12.951154530817911]  
Pd [6.738065507515291, 2.52927088967586, 12.951682087396721]  
Pd [9.466815966424686, 2.5274855079153022, 12.952349821991957]  
Pd [-0.0834553466784164, 4.892485984779299, 12.951836350223262]  
Pd [2.645205246666639, 4.893620918213767, 12.951274216449393]  
Pd [5.373536627391904, 4.893142014690238, 12.951282856459203]  
Pd [8.102879742451428, 4.890096161817006, 12.951965308146315]  
Pd [1.280669220302808, 7.256881132554258, 12.950748072636395]  
Pd [4.008809095885465, 7.25656035016786, 12.950981432932597]  
Pd [6.7383964807357755, 7.254126513302195, 12.951089417604985]  
Pd [9.466316701032982, 7.254146523040909, 12.951300209267702]