Parallelized Screening of Characterized and DFT-modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution

Eric M. Lopato\textsuperscript{a}, Emily A. Eikey\textsuperscript{b}, Zoe C. Simon\textsuperscript{b}, Seoin Back\textsuperscript{c}, Kevin Tran\textsuperscript{d}, Jacqueline Lewis\textsuperscript{a}, Jakub F. Kowalewski\textsuperscript{a}, Sadegh Yazdi\textsuperscript{e}, John R. Kitchin\textsuperscript{d}, Zachary W. Ulissi\textsuperscript{d}, Jill E. Millstone\textsuperscript{b}, and Stefan Bernhard\textsuperscript{a}*

a – Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, Pennsylvania 15213, United States
b – Department of Chemistry, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh, Pennsylvania 15260, United States
c - Department of Chemical and Biomolecular Engineering, Sogang University, Seoul 04107, Republic of Korea
d – Department of Chemical Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, Pennsylvania 15213, United States
e – Renewable and Sustainable Energy Institute, University of Colorado at Boulder, 4001 Discovery Drive, Boulder, Colorado 80309, United States
*Corresponding Author: Stefan Bernhard, bern@cmu.edu

Contents:

Page S3 – Figure S1. Time Resolved H\textsubscript{2} Evolution Plot for Pd/Sn and Ni/Sn
Page S4 – Figure S2. Time Resolved H\textsubscript{2} Evolution Plot for Pd/Pb and Pt/Sn
Page S5 – Figure S3. Time Resolved H\textsubscript{2} Evolution Plot for Pd/Mo and Pd/Ru
Page S6 – Figure S4. Time Resolved H\textsubscript{2} Evolution Plot for Pd/Ni and Mo/Sn
Page S7 – Figure S5. Fit Functions for All Tested Single-Metal WRCs
Page S8 – Table S1. Table of Studied MPIDs and Compositions
Page S8 – Table S2. Summary of Combined Activity Values for All Tested Metal Combinations
Page S9 – Figure S6. Linescans of 0.2 mM Pd/0.2 mM Sn

Page S10 – Figure S7. Bright-Field TEM Images and Size Distributions for Pd, Sn, and Pd/Sn at Various Compositions

Page S11 – Figure S8. Dark-Field Images and Linescans of Pd/Sn at Various Compositions

Page S12 – Figure S9. Bright-Field TEM Images of Non-Pd/Sn Systems Tested

Page S13 – Figure S10. XPS of Pd, Sn, and Pd/Sn at Various Compositions

Page S14 – Table S3. XPS Data for Experimental and Fitted Peaks

Page S14 – Figure S11. Full Reaction Time Scale Calibration

Page S15-S20 – Wolfram Mathematica Code Used to Analyze Images from the Parallel Photoreactor
Figure S1. Real time traces of H$_2$ evolved from in situ formed WRCs of (top) Pd/Sn and (bottom) Ni/Sn. Metal varying in the x-direction was tested at 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5, 0.6, and 0.65 mM, the metal varying in the y-direction was tested at 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, and 0.65 mM. Each graph spans 0-750 minutes on the x-axis and displays evolved H$_2$ on the y-axis with a range of 0-30 μmol.
**Figure S2.** Real time traces of H$_2$ evolved from *in situ* formed WRCs of (top) Pd/Pb and (bottom) Pt/Sn. Metal varying in the x-direction was tested at 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5, 0.6, and 0.65 mM, the metal varying in the y-direction was tested at 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, and 0.65 mM. Each graph spans 0-750 minutes on the x-axis and displays evolved H$_2$ on the y-axis with a range of 0-30 μmol.
**Figure S3.** Real time traces of H\textsubscript{2} evolved from *in situ* formed WRCs of (top) Pd/Mo and (bottom) Pd/Ru. Metal varying in the x-direction was tested at 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5, 0.6, and 0.65 mM, the metal varying in the y-direction was tested at 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, and 0.65 mM. Each graph spans 0-750 minutes on the x-axis and displays evolved H\textsubscript{2} on the y-axis with a range of 0-30 μmol.
Figure S4. Real time traces of H₂ evolved from in situ formed WRCs of (top) Pd/Ni and (bottom) Mo/Sn. Metal varying in the x-direction was tested at 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5, 0.6, and 0.65 mM, the metal varying in the y-direction was tested at 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, and 0.65 mM. Each graph spans 0-750 minutes on the x-axis and displays evolved H₂ on the y-axis with a range of 0-30 μmol.
Figure S5. Fourth order polynomial fit functions for WRCs containing only one metal component with measured values of H₂ evolution capacity expressed as maximum rate.
**Table S1.** All studied MPIDs, their formula, and ratios of Pd and Sn.

<table>
<thead>
<tr>
<th>MPIDs</th>
<th>Formula</th>
<th>Composition of Pd (r\textsubscript{pd})</th>
</tr>
</thead>
<tbody>
<tr>
<td>mp-117</td>
<td>Sn</td>
<td>0.00</td>
</tr>
<tr>
<td>mp-2128</td>
<td>Sn\textsubscript{3}Pd</td>
<td>0.20</td>
</tr>
<tr>
<td>mp-1371</td>
<td>Sn\textsubscript{2}Pd</td>
<td>0.25</td>
</tr>
<tr>
<td>mp-1573</td>
<td>Sn\textsubscript{2}Pd</td>
<td>0.33</td>
</tr>
<tr>
<td>mp-2369</td>
<td>SnPd</td>
<td>0.50</td>
</tr>
<tr>
<td>mp-1851</td>
<td>SnPd\textsubscript{2}</td>
<td>0.67</td>
</tr>
<tr>
<td>mp-718</td>
<td>SnPd\textsubscript{3}</td>
<td>0.75</td>
</tr>
<tr>
<td>mp-2</td>
<td>Pd</td>
<td>1.00</td>
</tr>
</tbody>
</table>

**Table S2.** Summary of combined activity values for each tested combination. Combined activity values are expressed as micromoles of hydrogen per hour.

<table>
<thead>
<tr>
<th>Names</th>
<th>Mean</th>
<th>Standard Deviation</th>
<th>Maximum</th>
<th>(x\ M_1\ Max)</th>
<th>(M_1) (mM) at Max</th>
<th>Minimum</th>
<th>(x\ M_1\ Min)</th>
<th>(M_1) (mM) at Min</th>
</tr>
</thead>
<tbody>
<tr>
<td>PtSn</td>
<td>5.41</td>
<td>5.37</td>
<td>17.99</td>
<td>33.33</td>
<td>0.15</td>
<td>-5.73</td>
<td>52.00</td>
<td>1.25</td>
</tr>
<tr>
<td>PdSn</td>
<td>-0.55</td>
<td>11.63</td>
<td>17.20</td>
<td>7.69</td>
<td>0.65</td>
<td>-29.28</td>
<td>86.67</td>
<td>0.75</td>
</tr>
<tr>
<td>PdRu</td>
<td>-9.61</td>
<td>12.85</td>
<td>14.14</td>
<td>11.11</td>
<td>0.45</td>
<td>-30.14</td>
<td>86.67</td>
<td>0.75</td>
</tr>
<tr>
<td>PdMo</td>
<td>-5.71</td>
<td>11.75</td>
<td>12.35</td>
<td>14.29</td>
<td>0.35</td>
<td>-29.72</td>
<td>76.47</td>
<td>0.85</td>
</tr>
<tr>
<td>PdNi</td>
<td>-11.17</td>
<td>11.34</td>
<td>5.63</td>
<td>14.29</td>
<td>0.35</td>
<td>-32.60</td>
<td>58.00</td>
<td>1.3</td>
</tr>
<tr>
<td>PdPb</td>
<td>-6.29</td>
<td>7.57</td>
<td>5.38</td>
<td>42.86</td>
<td>0.35</td>
<td>-23.68</td>
<td>50.00</td>
<td>1.3</td>
</tr>
<tr>
<td>NbSn</td>
<td>-0.48</td>
<td>0.15</td>
<td>0.26</td>
<td>76.47</td>
<td>0.85</td>
<td>-0.74</td>
<td>54.55</td>
<td>1.1</td>
</tr>
<tr>
<td>NiSn</td>
<td>-2.98</td>
<td>0.69</td>
<td>-1.41</td>
<td>20.00</td>
<td>0.25</td>
<td>-4.42</td>
<td>60.00</td>
<td>1.0</td>
</tr>
</tbody>
</table>
Figure S6. STEM-EDS map (as shown in Figure 9D) with particle linescans for 0.2 mM Pd/0.2 mM Sn system. In the linescans, Pd signal is represented in red and Sn signal is represented in blue (counts for both correspond to the left y-axis), and HAADF signal (image shown in Figure 9C) is represented in black (counts correspond to the right y-axis). Pd Lα and Sn Lα energies were used to generate linescans.
Figure S7. Representative bright-field TEM images and size histograms for (A and B) 0.2 mM Pd, (C and D) 0.2 mM Sn, (E and F) 0.6 mM Pd/0.2 mM Sn, and (G and H) 0.2 mM Pd/0.6 mM Sn systems.
Figure S8. Representative dark-field images and linescans for (A-C) 0.6 mM Pd/0.2 mM Sn and (D-F) 0.2 mM Pd/0.6 mM Sn systems, indicating that Pd and Sn elements can be found in the same particle. Pd Lα and Sn Lα energies were used to collect linescans.
Figure S9. Representative bright-field TEM images of the various bimetallic and monometallic systems explored in this work.
Figure S10. XPS of the Pd 3d and Sn 3d regions for 0.2 mM Pd system, 0.2 mM Sn system, 0.2 mM Pd/0.2 mM Sn system, 0.6 mM Pd/0.2 mM Sn system, and 0.2 mM Pd/0.6 mM Sn system. XPS shows the experimental spectrum in black, the fitted peaks in blue and orange, the overall fit in red, and the baseline in green. The black dotted lines act as guides for the eye for (left) Pd metal and (right) Sn metal. The binding energies for the experimental and fitted peaks can be found in Table S3.
Table S3. XPS data for experimental and fitted peaks.

<table>
<thead>
<tr>
<th>System</th>
<th>Experimental Peaks*</th>
<th>Fitted Peaks</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pd 3d_{5/2} (eV)</td>
<td>Sn 3d_{5/2} (eV)</td>
</tr>
<tr>
<td>0.2 mM Pd Only</td>
<td>335.2</td>
<td>---</td>
</tr>
<tr>
<td>0.2 mM Sn Only</td>
<td>---</td>
<td>487.3</td>
</tr>
<tr>
<td>0.2 mM Pd/0.2 mM Sn</td>
<td>335.5</td>
<td>486.3</td>
</tr>
<tr>
<td>0.6 mM Pd/0.2 mM Sn</td>
<td>335.6</td>
<td>485.6, 486.5</td>
</tr>
<tr>
<td>0.2 mM Pd/0.6 mM Sn</td>
<td>335.8</td>
<td>486.6</td>
</tr>
</tbody>
</table>

*Binding energies represent the center of the highest intensity peaks.

Figure S11. Full reaction time scale calibration testing. Each line represents a series of the average of 3 1 mL shell vials containing the same injected volume of H\textsubscript{2} as noted in the legend. H\textsubscript{2} was added to otherwise atmospheric pressure of air to each vial. Images were taken every 10 minutes for 750 minutes from the time of injection.
Following is the text version of the Mathematica program written for the analysis of data for photocatalytic systems of hydrogen evolution. A functional version of this code is attached in supporting information as a “.nb” file.

Questions

filename="PdcolSnrow"
Concentrations in mM, and volume in mL, and time in minutes
concPS = 0.25
concCat = 0.125
vialvol = 1.1
volSol = 0.44
headvol = vialvol - volSol
umolPS = concPS*volSol
umolCat = concCat*volSol
pictime = 10

Process mask

dimensions = 1944,2592
mc=MorphologicalComponents[mask]
dimensions = 1944,2592
centr=ComponentMeasurements[mc,"Centroid"]
dimensions = 96
masks=ComponentMeasurements[mc,"Mask"]
dimensions = 96
masks[[1,1]]
1
norms=Table[masks[[i,2]]//Flatten//Total,{i,1,96}]
ums=Show[Table[Graphics[Text[i,centr[[i,2]]]],{i,1,96}]]
ListPlot[centr[[All,2,2]]]

lbl=centr[[All,1]];  
acc=Accumulate[{12,12,12,12,12,12,12,12}];  
cc=centr[[All,2,1]];  
ccT=Table[cc[[If[i==1,1,acc[[i-1]]+1];;acc[[i]]]],{i,1,Length[acc]}];  
lblT=Table[lbl[[If[i==1,1,acc[[i-1]]+1];;acc[[i]]]],{i,1,Length[acc]}];  
ordT=Map[Ordering,ccT];  
ordAll=Table[lblT[[j]]||ordT[[j]]],{j,1,8}];  
ordM={ordAll[[1]],ordAll[[2]],ordAll[[3]],ordAll[[4]],ordAll[[5]],ordAll[[6]],ordAll[[7]],ordAll[[8]]}/Transpose;  
{nums,ordM}//TableForm

```math
\{(12, 11, 10, 9, 7, 4, 1, 2, 3, 5, 6, 8),
(23, 24, 22, 20, 21, 19, 14, 15, 16, 18, 13),
(36, 35, 34, 33, 32, 31, 30, 29, 26, 25, 27, 28),
(47, 48, 46, 44, 45, 43, 42, 37, 38, 39, 40, 41),
(60, 59, 58, 57, 51, 54, 52, 56, 55, 53, 50, 49),
```

```math
\{(13, 12, 11, 10, 9, 7, 4, 1, 2, 3, 5, 6, 8),
(23, 24, 22, 20, 21, 19, 14, 15, 16, 18, 13),
(36, 35, 34, 33, 32, 31, 30, 29, 26, 25, 27, 28),
(47, 48, 46, 44, 45, 43, 42, 37, 38, 39, 40, 41),
(60, 59, 58, 57, 51, 54, 52, 56, 55, 53, 50, 49),
```

```math
\{(13, 12, 11, 10, 9, 7, 4, 1, 2, 3, 5, 6, 8),
(23, 24, 22, 20, 21, 19, 14, 15, 16, 18, 13),
(36, 35, 34, 33, 32, 31, 30, 29, 26, 25, 27, 28),
(47, 48, 46, 44, 45, 43, 42, 37, 38, 39, 40, 41),
(60, 59, 58, 57, 51, 54, 52, 56, 55, 53, 50, 49),
```
{70, 71, 67, 68, 72, 69, 65, 66, 64, 63, 62, 61},
{80, 81, 79, 77, 82, 84, 83, 78, 76, 75, 73, 74},
{90, 91, 92, 93, 94, 96, 95, 89, 88, 87, 86, 85}
}}
ref={ordAll[[3,1]],ordAll[[4,1]],ordAll[[5,1]],ordAll[[6,1]]}
{36,47,60,70}
masks[[1,2]]//Dimensions
{1944,2592}

Directories

dir=FileNames["*",StringJoin["C:\\Users\\EMLop\\Documents\\",filename,"\"]]

{C:\Users\EMLop\Documents\PdcolSnrow\auxillary_data,C:\Users\EMLop\Documents\PdcolSnrow\images,C:\Users\EMLop\Documents\PdcolSnrow\PdcolSnrow.jpg,C:\Users\EMLop\Documents\PdcolSnrow\primary_data

pth=DirectoryName[dir[[1]]]
C:\Users\EMLop\Documents\PdcolSnrow

dirs=Map[FileNameTake,dir]
{auxillary_data,images,PdcolSnrow.jpg,primary_data}
{Range[Length[dirs]],dirs} // TableForm
{
{1, auxillary_data},
{2, images},
{3, PdcolSnrow.jpg},
{4, primary_data}
}
dirsOrd={2};
dirs=dirs[[dirsOrd]]
{images}
fnamsB=FileNames["*.jpg",StringJoin[pth,dirs[[1]]],10];
fnamsC=fnamsB[[1;;75]];
fnamsC//Dimensions
{75}
timesA=(Range[0,2000,pictime]);
timesC=timesA[[1;;75]];
timesC//Dimensions
{75}
ListPlot[timesC]

Processing and Graphic Generation

Monitor[dataB=Table[Total[ImageData[Import[fnamsC[[i]]]]][[1;;-1;;stepSize,1;;-1;;stepSize]],(3)]/3.,{i,1,Length[fnamsC]}],i];
Monitor[ resTabB = Table[ Flatten[ masks[[ ordM[[ i, j ]]]] ][ [ 1, 12 ], { i, 1, 8 } ], { j, 1, 8 } ], { k, 1, Length[ dataB ] }, { i, j, k } ];

Put[ { { timesC }, { resTabB } }, StringJoin[ "C:\Users\EMLop\Documents\", filename, "\auxillary_data\conc.res" ] ];

grB = Labeled[ GraphicsGrid[ Table[ ListLogPlot[ { ( timesC - timesC[[ 1 ]]) / resTabB[[ All, i, j ]] / resTabB[[ 1, i, j ]]], Joined -> True, PlotStyle -> { Gray, Thickness[ 0.05 ] }, PlotRange -> { All, { 0.5, 1.05 } }, Filling -> Axis, LabelingSize -> Medium, AspectRatio -> 1, Ticks -> { { 0, 250, 500, 750 }, { 0.5, 0.6, 0.75, 1 } }, { j, 1, 8 }, { i, 1, 12 } }, ImageSize -> 1500 ], "Normalized Darkness of the Tape", LabelStyle -> Directive[ Bold, FontFamily -> "Helvetica", 35 ] ];

grBA = Show[ Table[ ListLogPlot[ { ( timesC - timesC[[ 1 ]]) / resTabB[[ All, i, j ]] / resTabB[[ 1, i, j ]] }, [ [ 2 ;; 1 ] ], Joined -> True, PlotStyle -> { Blue, Thin }, PlotRange -> { All, { 0.5, 1.5 }, 0.5 }, { j, 2, Length[ resTabB ] }, { i, 1, 12 } ]; normresTabB = Flatten[ Transpose[ Table[ resTabB[[ All, i, j ]] / resTabB[[ 1, i, j ]] ], { j, 1, 8 }, { i, 1, 12 } ], 1 ];

h2perc = Transpose[ Table[ If[ ( ( normresTabB[[ k, i, j ]] - 1.0153 ) / ( -0.9355 ) ) < 0, normresTabB[[ k, i, j ]] = 0, ( ( normresTabB[[ k, i, j ]] - 1.0153 ) / ( -0.9355 ) ) ], { j, 1, 8 }, { i, 1, 12 } ];

percH = Labeled[ GraphicsGrid[ Table[ ListPlot[ { ( timesC - timesC[[ 1 ]]) / volH[[ All, i, j ]] ], Joined -> True, PlotStyle -> { Gray, Thickness[ 0.05 ] }, PlotRange -> { All, { 0.5, 1.1 } }, AspectRatio -> 1, Ticks -> { { 0, 20, 40, 60, 80, 100, 120, 140, 160, 180, 200, 220 }, Automatic }, { j, 1, 8 }, { i, 1, 12 } ]; volH = Table[ ( h2perc[[ k, i, j ]] * headvol ) / ( 1 - h2perc[[ k, i, j ]] ), { k, 1, Length[ h2perc ] }, { i, 1, 12 } ];

volumeH = Labeled[ GraphicsGrid[ Table[ ListPlot[ { ( timesC - timesC[[ 1 ]]) / mmolH[[ All, i, j ]] / mmolarH[[ 1, i, j ]] }, Joined -> True, PlotStyle -> { Gray, Thickness[ 0.05 ] }, PlotRange -> { All, { 0.5, 4 } }, AspectRatio -> 1, Ticks -> { { 0, 250, 500, 750, 1000 }, { 0, 4, 8, 12 } }, { j, 1, 8 }, { i, 1, 12 } ]; mmolH = Table[ ( volH[[ k, i ]] ) / ( 0.08206 * 298 ) * 1000 ), { k, 1, Length[ volH ] }, { i, 1, 12 } ];

mmolarH = Labeled[ GraphicsGrid[ Table[ ListPlot[ { timesC[[ All, i, j ]] }, { i, 1, 12 } ]; oren = Transpose[ Table[ MovingAverage[ mmolH[[ All, i, j ]], 4 ], { i, 1, 12 } ], { j, 1, 8 } ];

doren = Table[ oren[[ p + 1, i, j ]], p, Length[ oren ] - 1 ], { i, 1, 12 } ];

ddoren = Transpose[ Table[ MovingAverage[ doren[[ All, i, j ]], 4 ], { i, 1, 12 } ], { j, 1, 8 } ];

gausdoren = Transpose[ Table[ GaussianFilter[ doren[[ All, i, j ]], 12 ], { i, 1, 12 }, { j, 1, 8 } ];

secondderiv = Table[ gausdoren[[ k + 1, i, j ]], k, 1, Length[ gausdoren ] ];
integTab = Table[rng = Head[derivTab[[i, j]]][[1]] // Flatten;
  (NIntegrate[derivTab[[i, j]], {x, rng[[1]], rng[[2]]}]/Differences[rng][[1]], {i, 1, 8}, {j, 1, 12}]);
integTabexp = Flatten[Transpose[Table[If[(integTab[[j, i]]*60) < 0, integTab[[j, i]] = 0, integTab[[j, i]]*60], {i, 1, 8}, {j, 1, 12}]]];
ListContourPlot[integTab[[1;;1;;1-1]], ColorFunction -> "SunsetColors", InterpolationOrder -> 0];

ExportStringJoin["C:\\ Users\\EMLop\\Documents\\\auxillary_data\\"]

grGAll = {grB};
grGAlls = {"grayscale"};
grGAllAll = {grBA};
Do[Export[StringJoin[pthExp, filename, grGAlls[[j]], ".png"], grGAll[[j]], {j, 1, 1}]
Do[Export[StringJoin[pthExp, filename, "composite", ",.png"], grGAllAll[[j]], {j, 1, 1}]
Do[Export[StringJoin[pthExp, filename, "darknessdata", ",.csv"], resTabB[[j]], {j, All, All}]
Do[Export[StringJoin[pthExp, filename, "darknessdatas", ",.xls"], resTabB[[j]], {j, All, All}]
Expand[StringJoin[pthExp, filename, "percH", ",.jpg"], percH];
Expand[StringJoin[pthExp, filename, "volH", ",.jpg"], volumeH];
Expand[StringJoin[pthExp, filename, "mmolH", ",.jpg"], mmolarH];
Expand[StringJoin[pthExp, filename, "running_average_umolH", ",.jpg"], averagegrid2];
Expand[StringJoin[pthExp, filename, "derivative_umolH", ",.jpg"], gausavggrid];
checkresTabB = Transpose[resTabB, {3, 2, 1}];
expresTabB = Flatten[Transpose[resTabB, {3, 2, 1}], 1];
Do[Export[StringJoin[pthExp, filename, "darknessdatas2", ",.xls"], expresTabB[[j]], {j, All, All}]
{96, 161}

checknormresTabB = Transpose[normresTabB, {3, 2, 1}];
expnormresTabB = Flatten[Transpose[normresTabB, {3, 2, 1}], 1];
Do[Export[StringJoin[pthExp, filename, "normresTabB", ",.xls"], expnormresTabB[[j]], {j, All, All}]
{96, 160}

checkmmolH = Transpose[mmolH, {3, 2, 1}];
expmmolH = Flatten[Transpose[mmolH, {3, 2, 1}], 1];
Do[Export[StringJoin[pthExp, filename, "mmolH", ",.xls"], expmmolH[[j]], {j, All, All}]
{96, 160}
   Export[StringJoin[pthExp, filename, "maxH", ",.xls"], maxlistexp];
   Export[StringJoin[pthExp, filename, "maxderiv", ",.xls"], maxlistderivperhour];
   Export[StringJoin[pthExp, filename, "TONPS", ",.xls"], TONPS];
   Export[StringJoin[pthExp, filename, "TONCat", ",.xls"], TONCat];
   Export[StringJoin[pthExp, filename, "TOFPS", ",.xls"], TOFPS];
   Export[StringJoin[pthExp, filename, "TOFCat", ",.xls"], TOFCat];
   Export[StringJoin[pthExp, filename, "avgderiv", ",.xls"], integTabexp];