

Electronic supplementary information

Can surface energy be a parameter to define morphological change of rock-salt crystals with additives? A first principle study

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Clean (100) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.09297732592380 | -0.03819235142316 | 5.51855138770084 |
| Na | -0.09297732592380 | 10.58206825561204 | 5.51855138770084 |
| Na | 10.52728328111139 | -0.03819235142316 | 5.51855138770084 |
| Na | 10.52728328111139 | 10.58206825561204 | 5.51855138770084 |
| Na | -0.09297732592380 | -0.03819235142316 | 16.13881199284631 |
| Na | -0.09297732592380 | 10.58206825561204 | 16.13881199284631 |
| Na | 10.52728328111139 | -0.03819235142316 | 16.13881199284631 |
| Na | 10.52728328111139 | 10.58206825561204 | 16.13881199284631 |
| Na | -0.09297732592380 | -0.03819235142316 | 26.75907259988151 |
| Na | -0.09297732592380 | 10.58206825561204 | 26.75907259988151 |
| Na | 10.52728328111139 | -0.03819235142316 | 26.75907259988151 |
| Na | 10.52728328111139 | 10.58206825561204 | 26.75907259988151 |
| Na | -0.09297155092076 | -0.03818885165037 | 36.98699204640806 |
| Na | -0.09296972733505 | 10.58206430797416 | 36.98698409444052 |
| Na | 10.52728453588954 | -0.03818853228666 | 36.98697871061079 |
| Na | 10.52729646384084 | 10.58207293835338 | 36.98698600873308 |
| Na | 5.21715297759380 | 5.27193795209444 | 5.51855138770084 |
| Na | 5.21715297759380 | 15.89219855912964 | 5.51855138770084 |
| Na | 15.83741358273927 | 5.27193795209444 | 5.51855138770084 |
| Na | 15.83741358273927 | 15.89219855912964 | 5.51855138770084 |
| Na | 5.21715297759380 | 5.27193795209444 | 16.13881199284631 |
| Na | 5.21715297759380 | 15.89219855912964 | 16.13881199284631 |
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| Na | 5.21715297759380 | 5.27193795209444 | 26.75907259988151 |
| Na | 5.21715297759380 | 15.89219855912964 | 26.75907259988151 |
| Na | 15.83741358273927 | 5.27193795209444 | 26.75907259988151 |
| Na | 15.83741358273927 | 15.89219855912964 | 26.75907259988151 |
| Na | 5.21714088901577 | 5.27193326368392 | 36.98698703296465 |
| Na | 5.21715174171291 | 15.89219470975752 | 36.98697876730257 |
| Na | 15.83740571202996 | 5.27194200555698 | 36.98698224439865 |
| Na | 15.83740780962595 | 15.89219404835338 | 36.98699117335459 |
| Na | -0.09297732592380 | 5.27193795209444 | 0.20842108418324 |
| Na | -0.09297732592380 | 15.89219855912964 | 0.20842108418324 |
| Na | 10.52728328111139 | 5.27193795209444 | 0.20842108418324 |
| Na | 10.52728328111139 | 15.89219855912964 | 0.20842108418324 |
| Na | -0.09297732592380 | 5.27193795209444 | 10.82868169121844 |
| Na | -0.09297732592380 | 15.89219855912964 | 10.82868169121844 |
| Na | 10.52728328111139 | 5.27193795209444 | 10.82868169121844 |
| Na | 10.52728328111139 | 15.89219855912964 | 10.82868169121844 |
| Na | -0.09297732592380 | 5.27193795209444 | 21.44894229636391 |
| Na | -0.09297732592380 | 15.89219855912964 | 21.44894229636391 |
| Na | 10.52728328111139 | 5.27193795209444 | 21.44894229636391 |
| Na | 10.52728328111139 | 15.89219855912964 | 21.44894229636391 |
| Na | -0.09297950666775 | 5.27193794642526 | 31.94316037806215 |
| Na | -0.09297799866630 | 15.89219831535497 | 31.94316750610909 |
| Na | 10.52728123642773 | 5.27193891585476 | 31.94316236227458 |
| Na | 10.52728270852438 | 15.89219929045365 | 31.94316198243962 |
| Na | 5.21715297759380 | -0.03819235142316 | 0.20842108418324 |
| Na | 5.21715297759380 | 10.58206825561204 | 0.20842108418324 |
| Na | 15.83741358273927 | -0.03819235142316 | 0.20842108418324 |
| Na | 15.83741358273927 | 10.58206825561204 | 0.20842108418324 |
| Na | 5.21715297759380 | -0.03819235142316 | 10.82868169121844 |
| Na | 5.21715297759380 | 10.58206825561204 | 10.82868169121844 |
| Na | 15.83741358273927 | -0.03819235142316 | 10.82868169121844 |
| Na | 15.83741358273927 | 10.58206825561204 | 10.82868169121844 |
| Na | 5.21715297759380 | -0.03819235142316 | 21.44894229636391 |
| Na | 5.21715297759380 | 10.58206825561204 | 21.44894229636391 |
| Na | 15.83741358273927 | -0.03819235142316 | 21.44894229636391 |
| Na | 15.83741358273927 | 10.58206825561204 | 21.44894229636391 |
| Na | 5.21715362010068 | -0.03819314510813 | 31.94316205802867 |
| Na | 5.21715503928500 | 10.58206730319007 | 31.94316259660062 |
| Na | 15.83741427059958 | -0.03819211898684 | 31.94316746831457 |
| Na | 15.83741572190924 | 10.58206836143670 | 31.94315816897230 |
| Cl | 5.21715297759380 | 5.27193795209444 | 0.20842108418324 |
| Cl | 5.21715297759380 | 15.89219855912964 | 0.20842108418324 |
| Cl | 15.83741358273927 | 5.27193795209444 | 0.20842108418324 |
| Cl | 15.83741358273927 | 15.89219855912964 | 0.20842108418324 |

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| C1 | 5.21715297759380 | 15.89219855912964 | 10.82868169121844 |
| C1 | 15.83741358273927 | 5.27193795209444 | 10.82868169121844 |
| C1 | 15.83741358273927 | 15.89219855912964 | 10.82868169121844 |
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| C1 | 5.21715297759380 | 15.89219855912964 | 21.44894229636391 |
| C1 | 15.83741358273927 | 5.27193795209444 | 21.44894229636391 |
| C1 | 15.83741358273927 | 15.89219855912964 | 21.44894229636391 |
| C1 | 5.21715099905054 | 5.27193695242932 | 31.90985423289887 |
| C1 | 5.21715193257525 | 15.89219780134946 | 31.90985130571310 |
| C1 | 15.83741131695764 | 5.27193731714646 | 31.90985207294191 |
| C1 | 15.83741336731049 | 15.89219951722078 | 31.90985653647502 |
| C1 | -0.09297732592380 | -0.03819235142316 | 0.20842108418324 |
| C1 | -0.09297732592380 | 10.58206825561204 | 0.20842108418324 |
| C1 | 10.52728328111139 | -0.03819235142316 | 0.20842108418324 |
| C1 | 10.52728328111139 | 10.58206825561204 | 0.20842108418324 |
| C1 | -0.09297732592380 | -0.03819235142316 | 10.82868169121844 |
| C1 | -0.09297732592380 | 10.58206825561204 | 10.82868169121844 |
| C1 | 10.52728328111139 | -0.03819235142316 | 10.82868169121844 |
| C1 | 10.52728328111139 | 10.58206825561204 | 10.82868169121844 |
| C1 | -0.09297732592380 | -0.03819235142316 | 21.44894229636391 |
| C1 | -0.09297732592380 | 10.58206825561204 | 21.44894229636391 |
| C1 | 10.52728328111139 | -0.03819235142316 | 21.44894229636391 |
| C1 | 10.52728328111139 | 10.58206825561204 | 21.44894229636391 |
| C1 | -0.09297702167790 | -0.03819311487251 | 31.90985709772368 |
| C1 | -0.09297491841272 | 10.58206878662508 | 31.90985285717825 |
| C1 | 10.52728433557857 | -0.03819158041490 | 31.90985125846995 |
| C1 | 10.52728509902793 | 10.58206919291620 | 31.90985359795909 |
| C1 | 5.21715297759380 | -0.03819235142316 | 5.51855138770084 |
| C1 | 5.21715297759380 | 10.58206825561204 | 5.51855138770084 |
| C1 | 15.83741358273927 | -0.03819235142316 | 5.51855138770084 |
| C1 | 15.83741358273927 | 10.58206825561204 | 5.51855138770084 |
| C1 | 5.21715297759380 | -0.03819235142316 | 16.13881199284631 |
| C1 | 5.21715297759380 | 10.58206825561204 | 16.13881199284631 |
| C1 | 15.83741358273927 | -0.03819235142316 | 16.13881199284631 |
| C1 | 15.83741358273927 | 10.58206825561204 | 16.13881199284631 |
| C1 | 5.21715297759380 | -0.03819235142316 | 26.75907259988151 |
| C1 | 5.21715297759380 | 10.58206825561204 | 26.75907259988151 |
| C1 | 15.83741358273927 | -0.03819235142316 | 26.75907259988151 |
| C1 | 15.83741358273927 | 10.58206825561204 | 26.75907259988151 |
| C1 | 5.21715520180144 | -0.03819806973441 | 37.14933722916852 |
| C1 | 5.21716239409908 | 10.58206598227151 | 37.14933863323504 |
| C1 | 15.83741623969420 | -0.03819273125811 | 37.14935141723227 |
| C1 | 15.83742429559667 | 10.58206895670043 | 37.14932578309738 |
| C1 | -0.09297732592380 | 5.27193795209444 | 5.51855138770084 |
| C1 | -0.09297732592380 | 15.89219855912964 | 5.51855138770084 |
| C1 | 10.52728328111139 | 5.27193795209444 | 5.51855138770084 |
| C1 | 10.52728328111139 | 15.89219855912964 | 5.51855138770084 |
| C1 | -0.09297732592380 | 5.27193795209444 | 16.13881199284631 |
| C1 | -0.09297732592380 | 15.89219855912964 | 16.13881199284631 |
| C1 | 10.52728328111139 | 5.27193795209444 | 16.13881199284631 |
| C1 | 10.52728328111139 | 15.89219855912964 | 16.13881199284631 |
| C1 | -0.09297732592380 | 5.27193795209444 | 26.75907259988151 |
| C1 | -0.09297732592380 | 15.89219855912964 | 26.75907259988151 |
| C1 | 10.52728328111139 | 5.27193795209444 | 26.75907259988151 |
| C1 | 10.52728328111139 | 15.89219855912964 | 26.75907259988151 |
| C1 | -0.09298665928113 | 5.27193596410256 | 37.14933157510796 |
| C1 | -0.09297989217188 | 15.89219864416731 | 37.14935145691652 |
| C1 | 10.52727422365408 | 5.27194012716921 | 37.14933821182611 |
| C1 | 10.52728097753525 | 15.89220434736076 | 37.14933707988016 |

Clean (110) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.17726733140716 | 7.48982612461360 | 4.11318466777784 |
| Na | -0.17726733140716 | 22.50914271042150 | 4.11318466777784 |
| Na | 10.44299327373831 | 7.48982612461360 | 4.11318466777784 |
| Na | 10.44299327373831 | 22.50914271042150 | 4.11318466777784 |
| Na | -0.17726733140716 | -0.01983216734548 | 11.62284296162665 |

| | | | |
|----|-------------------|-------------------|--------------------|
| Na | -0.17726733140716 | 14.99948441846241 | 11.62284296162665 |
| Na | 10.44299327373831 | -0.01983216734548 | 11.62284296162665 |
| Na | 10.44299327373831 | 14.99948441846241 | 11.62284296162665 |
| Na | -0.17726733140716 | 7.48982612461360 | 19.13250125358573 |
| Na | -0.17726733140716 | 22.50914271042150 | 19.13250125358573 |
| Na | 10.44299327373831 | 7.48982612461360 | 19.13250125358573 |
| Na | 10.44299327373831 | 22.50914271042150 | 19.13250125358573 |
| Na | -0.17726714810373 | -0.01984905204841 | 26.09032719517104 |
| Na | -0.17726733896606 | 14.99947177619464 | 26.09034025506829 |
| Na | 10.44299348349791 | -0.01984905204841 | 26.09032720650940 |
| Na | 10.44299327373831 | 14.99947179698163 | 26.09034027585528 |
| Na | 5.13286297211044 | 11.24465527153801 | 0.35835552274316 |
| Na | 5.13286297211044 | 26.26397185734590 | 0.35835552274316 |
| Na | 15.75312357725591 | 11.24465527153801 | 0.35835552274316 |
| Na | 15.75312357725591 | 26.26397185734590 | 0.35835552274316 |
| Na | 5.13286297211044 | 3.73499697957892 | 7.86801381470224 |
| Na | 5.13286297211044 | 18.75431356538682 | 7.86801381470224 |
| Na | 15.75312357725591 | 3.73499697957892 | 7.86801381470224 |
| Na | 15.75312357725591 | 18.75431356538682 | 7.86801381470224 |
| Na | 5.13286297211044 | 11.24465527153801 | 15.37767210666132 |
| Na | 5.13286297211044 | 26.26397185734590 | 15.37767210666132 |
| Na | 15.75312357725591 | 11.24465527153801 | 15.37767210666132 |
| Na | 15.75312357725591 | 26.26397185734590 | 15.37767210666132 |
| Na | 5.13286284738851 | 3.73497967913625 | 22.84911503600222 |
| Na | 5.13286289841112 | 18.75432572388470 | 22.849114444073850 |
| Na | 15.75312337316549 | 3.73497969614379 | 22.84911498308989 |
| Na | 15.75312339017302 | 18.75432569931827 | 22.84911440483370 |
| Na | 5.13286297211044 | 3.73499697957892 | 0.35835552274316 |
| Na | 5.13286297211044 | 18.75431356538682 | 0.35835552274316 |
| Na | 15.75312357725591 | 3.73499697957892 | 0.35835552274316 |
| Na | 15.75312357725591 | 18.75431356538682 | 0.35835552274316 |
| Na | 5.13286297211044 | 11.24465527153801 | 7.86801381470224 |
| Na | 5.13286297211044 | 26.26397185734590 | 7.86801381470224 |
| Na | 15.75312357725591 | 11.24465527153801 | 7.86801381470224 |
| Na | 15.75312357725591 | 26.26397185734590 | 7.86801381470224 |
| Na | 5.13286297211044 | 3.73499697957892 | 15.37767210666132 |
| Na | 5.13286297211044 | 18.75431356538682 | 15.37767210666132 |
| Na | 15.75312357725591 | 3.73499697957892 | 15.37767210666132 |
| Na | 15.75312357725591 | 18.75431356538682 | 15.37767210666132 |
| Na | 5.13286301557414 | 11.24466342570624 | 22.84911295163431 |
| Na | 5.13286296077208 | 26.26399317534632 | 22.84909006138176 |
| Na | 15.75312354702029 | 11.24466343137542 | 22.84911288549389 |
| Na | 15.75312350355659 | 26.26399318101550 | 22.84909003681532 |
| Na | -0.17726733140716 | -0.01983216734548 | 4.11318466777784 |
| Na | 10.44299327373831 | 14.99948441846241 | 4.11318466777784 |
| Na | 10.44299327373831 | -0.01983216734548 | 4.11318466777784 |
| Na | 10.44299327373831 | 14.99948441846241 | 4.11318466777784 |
| Na | -0.17726733140716 | 7.48982612461360 | 11.62284296162665 |
| Na | -0.17726733140716 | 22.50914271042150 | 11.62284296162665 |
| Na | 10.44299327373831 | 7.48982612461360 | 11.62284296162665 |
| Na | 10.44299327373831 | 22.50914271042150 | 11.62284296162665 |
| Na | -0.17726733140716 | -0.01983216734548 | 19.13250125358573 |
| Na | -0.17726733140716 | 14.99948441846241 | 19.13250125358573 |
| Na | 10.44299327373831 | -0.01983216734548 | 19.13250125358573 |
| Na | 10.44299327373831 | 14.99948441846241 | 19.13250125358573 |
| Na | -0.17726725581811 | 7.48981782682619 | 26.09037079871165 |
| Na | -0.17726722747222 | 22.50917784798906 | 26.09029342765491 |
| Na | 10.44299335310681 | 7.48981787784879 | 26.09037081949864 |
| Na | 10.44299340034996 | 22.50917777617947 | 26.09029346544944 |
| Cl | 5.13286297211044 | -0.01983216734548 | 4.11318466777784 |
| Cl | 5.13286297211044 | 14.99948441846241 | 4.11318466777784 |
| Cl | 15.75312357725591 | -0.01983216734548 | 4.11318466777784 |
| Cl | 15.75312357725591 | 14.99948441846241 | 4.11318466777784 |
| Cl | 5.13286297211044 | 7.48982612461360 | 11.62284296162665 |
| Cl | 5.13286297211044 | 22.50914271042150 | 11.62284296162665 |
| Cl | 15.75312357725591 | 7.48982612461360 | 11.62284296162665 |
| Cl | 15.75312357725591 | 22.50914271042150 | 11.62284296162665 |
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| Cl | 5.13286297211044 | 14.99948441846241 | 19.13250125358573 |
| Cl | 15.75312357725591 | -0.01983216734548 | 19.13250125358573 |
| Cl | 15.75312357725591 | 14.99948441846241 | 19.13250125358573 |

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| C1 | 5.13286303069195 | 7.48982178958187 | 26.33375725294934 |
| C1 | 5.13286306470702 | 22.50917335799979 | 26.33377697602090 |
| C1 | 15.75312367363194 | 7.48982180847913 | 26.33375718869865 |
| C1 | 15.75312371142646 | 22.50917332965390 | 26.33377692310857 |
| C1 | -0.17726733140716 | 3.73499697957892 | 0.35835552274316 |
| C1 | -0.17726733140716 | 18.75431356538682 | 0.35835552274316 |
| C1 | 10.44299327373831 | 3.73499697957892 | 0.35835552274316 |
| C1 | 10.44299327373831 | 18.75431356538682 | 0.35835552274316 |
| C1 | -0.17726733140716 | 11.24465527153801 | 7.86801381470224 |
| C1 | -0.17726733140716 | 26.26397185734590 | 7.86801381470224 |
| C1 | 10.44299327373831 | 11.24465527153801 | 7.86801381470224 |
| C1 | 10.44299327373831 | 26.26397185734590 | 7.86801381470224 |
| C1 | -0.17726733140716 | 3.73499697957892 | 15.37767210666132 |
| C1 | -0.17726733140716 | 18.75431356538682 | 15.37767210666132 |
| C1 | 10.44299327373831 | 3.73499697957892 | 15.37767210666132 |
| C1 | 10.44299327373831 | 18.75431356538682 | 15.37767210666132 |
| C1 | -0.17726731250990 | 11.24464122520372 | 22.74602511284108 |
| C1 | -0.17726733329689 | 26.26401883971682 | 22.74599806897051 |
| C1 | 10.44299327184858 | 11.24464125732906 | 22.74602517709177 |
| C1 | 10.44299319059036 | 26.26401879814285 | 22.74599817668490 |
| C1 | -0.17726733140716 | 11.24465527153801 | 0.35835552274316 |
| C1 | -0.17726733140716 | 26.26397185734590 | 0.35835552274316 |
| C1 | 10.44299327373831 | 11.24465527153801 | 0.35835552274316 |
| C1 | 10.44299327373831 | 26.26397185734590 | 0.35835552274316 |
| C1 | -0.17726733140716 | 3.73499697957892 | 7.86801381470224 |
| C1 | -0.17726733140716 | 18.75431356538682 | 7.86801381470224 |
| C1 | 10.44299327373831 | 3.73499697957892 | 7.86801381470224 |
| C1 | 10.44299327373831 | 18.75431356538682 | 7.86801381470224 |
| C1 | -0.17726733140716 | 11.24465527153801 | 15.37767210666132 |
| C1 | -0.17726733140716 | 26.26397185734590 | 15.37767210666132 |
| C1 | 10.44299327373831 | 11.24465527153801 | 15.37767210666132 |
| C1 | 10.44299327373831 | 26.26397185734590 | 15.37767210666132 |
| C1 | -0.17726746179826 | 3.73499806050227 | 22.74602542086644 |
| C1 | -0.17726743156264 | 18.75430866154753 | 22.74602241809163 |
| C1 | 10.44299308098624 | 3.73499808695843 | 22.74602552480138 |
| C1 | 10.44299311689104 | 18.75430864642971 | 22.74602247478341 |
| C1 | 5.13286297211044 | 7.48982612461360 | 4.11318466777784 |
| C1 | 5.13286297211044 | 22.50914271042150 | 4.11318466777784 |
| C1 | 15.75312357725591 | 7.48982612461360 | 4.11318466777784 |
| C1 | 15.75312357725591 | 22.50914271042150 | 4.11318466777784 |
| C1 | 5.13286297211044 | -0.01983216734548 | 11.62284296162665 |
| C1 | 5.13286297211044 | 14.99948441846241 | 11.62284296162665 |
| C1 | 15.75312357725591 | -0.01983216734548 | 11.62284296162665 |
| C1 | 15.75312357725591 | 14.99948441846241 | 11.62284296162665 |
| C1 | 5.13286297211044 | 7.48982612461360 | 19.13250125358573 |
| C1 | 5.13286297211044 | 22.50914271042150 | 19.13250125358573 |
| C1 | 15.75312357725591 | 7.48982612461360 | 19.13250125358573 |
| C1 | 15.75312357725591 | 22.50914271042150 | 19.13250125358573 |
| C1 | 5.13286314974469 | -0.01987783446702 | 26.33376016879675 |
| C1 | 5.13286294565427 | 14.99949889754398 | 26.33378024713682 |
| C1 | 15.75312379079496 | -0.01987779100332 | 26.33376012155359 |
| C1 | 15.75312359615317 | 14.99949887108782 | 26.33378020367312 |

Clean (111) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 0.00021954838120 | -0.01509695965161 | 3.29706134427511 |
| Na | 0.00021954838120 | 15.00421962426656 | 3.29706134427511 |
| Na | 13.00732925855620 | 7.49456133230747 | 3.29706134427511 |
| Na | 13.00732925855620 | 22.51387791811536 | 3.29706134427511 |
| Na | 8.67162602120129 | -0.01509695965161 | 9.42867166455839 |
| Na | 8.67162602120129 | 15.00421962426656 | 9.42867166455839 |
| Na | 21.67873573137628 | 7.49456133230747 | 9.42867166455839 |
| Na | 21.67873573137628 | 22.51387791811536 | 9.42867166455839 |
| Na | 4.33592278573611 | 7.49456133230747 | 15.56028198484167 |
| Na | 4.33592278573611 | 22.51387791811536 | 15.56028198484167 |
| Na | 17.34303249591110 | -0.01509695965161 | 15.56028198484167 |
| Na | 17.34303249591110 | 15.00421962426656 | 15.56028198484167 |
| Na | 0.01147971582302 | -0.01628535738901 | 21.50769696184354 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 0.01138122518711 | 15.00557982456489 | 21.49682293158948 |
| Na | 13.01470654525775 | 7.49609042120905 | 21.50416882049146 |
| Na | 13.01861825565977 | 22.51789326109808 | 21.49712327332143 |
| Na | 0.00021954838120 | 7.49456133230747 | 3.29706134427511 |
| Na | 0.00021954838120 | 22.51387791811536 | 3.29706134427511 |
| Na | 13.00732925855620 | -0.01509695965161 | 3.29706134427511 |
| Na | 13.00732925855620 | 15.00421962426656 | 3.29706134427511 |
| Na | 8.67162602120129 | 7.49456133230747 | 9.42867166455839 |
| Na | 8.67162602120129 | 22.51387791811536 | 9.42867166455839 |
| Na | 21.67873573137628 | -0.01509695965161 | 9.42867166455839 |
| Na | 21.67873573137628 | 15.00421962426656 | 9.42867166455839 |
| Na | 4.33592278573611 | -0.01509695965161 | 15.56028198484167 |
| Na | 4.33592278573611 | 15.00421962426656 | 15.56028198484167 |
| Na | 17.34303249591110 | 7.49456133230747 | 15.56028198484167 |
| Na | 17.34303249591110 | 22.51387791811536 | 15.56028198484167 |
| Na | 0.00800343800444 | 7.49540177099403 | 21.50235305068810 |
| Na | 0.00923770884353 | 22.51827196599298 | 21.48939231114750 |
| Na | 13.01760219716552 | -0.01126373713446 | 21.50271630707193 |
| Na | 13.02004296175938 | 15.00781780075855 | 21.49294737542768 |
| Na | 6.50377440441356 | 3.73973218538307 | 3.29706134427511 |
| Na | 6.50377440441356 | 18.75904877119096 | 3.29706134427511 |
| Na | 19.51088411458856 | 11.24939047923188 | 3.29706134427511 |
| Na | 19.51088411458856 | 26.26870706503977 | 3.29706134427511 |
| Na | 2.16807116705866 | 11.24939047923188 | 9.42867166455839 |
| Na | 2.16807116705866 | 26.26870706503977 | 9.42867166455839 |
| Na | 15.17518087723365 | 3.73973218538307 | 9.42867166455839 |
| Na | 15.17518087723365 | 18.75904877119096 | 9.42867166455839 |
| Na | 10.83947763987874 | 11.24939047923188 | 15.56028198484167 |
| Na | 10.83947763987874 | 26.26870706503977 | 15.56028198484167 |
| Na | 23.84658735005374 | 3.73973218538307 | 15.56028198484167 |
| Na | 23.84658735005374 | 18.75904877119096 | 15.56028198484167 |
| Na | 6.50895190628644 | 3.74289992194804 | 21.48958041826544 |
| Na | 6.50927792561697 | 18.75649459090425 | 21.50178046934140 |
| Na | 19.52368615492918 | 11.24498089591578 | 21.49308784821918 |
| Na | 19.52428755837873 | 26.26299086271990 | 21.50240462131405 |
| Na | 6.50377440441356 | 11.24939047923188 | 3.29706134427511 |
| Na | 6.50377440441356 | 26.26870706503977 | 3.29706134427511 |
| Na | 19.51088411458856 | 3.73973218538307 | 3.29706134427511 |
| Na | 19.51088411458856 | 18.75904877119096 | 3.29706134427511 |
| Na | 2.16807116705866 | 3.73973218538307 | 9.42867166455839 |
| Na | 2.16807116705866 | 18.75904877119096 | 9.42867166455839 |
| Na | 15.17518087723365 | 11.24939047923188 | 9.42867166455839 |
| Na | 15.17518087723365 | 26.26870706503977 | 9.42867166455839 |
| Na | 10.83947763987874 | 3.73973218538307 | 15.56028198484167 |
| Na | 10.83947763987874 | 18.75904877119096 | 15.56028198484167 |
| Na | 23.84658735005374 | 11.24939047923188 | 15.56028198484167 |
| Na | 23.84658735005374 | 26.26870706503977 | 15.56028198484167 |
| Na | 6.51474460094040 | 11.25196730032729 | 21.50145604304999 |
| Na | 6.51470899283103 | 26.26918311350682 | 21.50014646851455 |
| Na | 19.52083899150405 | 3.73560433566577 | 21.49586899784158 |
| Na | 19.51566593237730 | 18.75660853194096 | 21.50491902664528 |
| Cl | 8.67162602120129 | -0.01509695965161 | 0.23125618507833 |
| Cl | 8.67162602120129 | 15.00421962426656 | 0.23125618507833 |
| Cl | 21.67873573137628 | 7.49456133230747 | 0.23125618507833 |
| Cl | 21.67873573137628 | 22.51387791811536 | 0.23125618507833 |
| Cl | 4.33592278573611 | 7.49456133230747 | 6.36286650347188 |
| Cl | 4.33592278573611 | 22.51387791811536 | 6.36286650347188 |
| Cl | 17.34303249591110 | -0.01509695965161 | 6.36286650347188 |
| Cl | 17.34303249591110 | 15.00421962426656 | 6.36286650347188 |
| Cl | 0.00021954838120 | -0.01509695965161 | 12.49447682375516 |
| Cl | 0.00021954838120 | 15.00421962426656 | 12.49447682375516 |
| Cl | 13.00732925855620 | 7.49456133230747 | 12.49447682375516 |
| Cl | 13.00732925855620 | 22.51387791811536 | 12.49447682375516 |
| Cl | 8.67339220459113 | -0.01570850148183 | 18.85179820937217 |
| Cl | 8.67122051243103 | 15.00586334584460 | 18.85097692305989 |
| Cl | 21.68236028655526 | 7.49087424609102 | 18.85057928877840 |
| Cl | 21.67850117290047 | 22.50765506510357 | 18.85117694301132 |
| Cl | 8.67162602120129 | 7.49456133230747 | 0.23125618507833 |
| Cl | 8.67162602120129 | 22.51387791811536 | 0.23125618507833 |
| Cl | 21.67873573137628 | -0.01509695965161 | 0.23125618507833 |
| Cl | 21.67873573137628 | 15.00421962426656 | 0.23125618507833 |

| | | | |
|----|-------------------|-------------------|-------------------|
| C1 | 4.33592278573611 | -0.01509695965161 | 6.36286650347188 |
| C1 | 4.33592278573611 | 15.00421962426656 | 6.36286650347188 |
| C1 | 17.34303249591110 | 7.49456133230747 | 6.36286650347188 |
| C1 | 17.34303249591110 | 22.51387791811536 | 6.36286650347188 |
| C1 | 0.00021954838120 | 7.49456133230747 | 12.49447682375516 |
| C1 | 0.00021954838120 | 22.51387791811536 | 12.49447682375516 |
| C1 | 13.00732925855620 | -0.01509695965161 | 12.49447682375516 |
| C1 | 13.00732925855620 | 15.00421962426656 | 12.49447682375516 |
| C1 | 8.67519307957318 | 7.49770253522792 | 18.85203224250412 |
| C1 | 8.67001004080276 | 22.51041775588119 | 18.85233951764122 |
| C1 | 21.68206702940655 | -0.01889961773841 | 18.85321932499214 |
| C1 | 21.67790632113139 | 15.00636629267331 | 18.85173916487940 |
| C1 | 2.16807116705866 | 11.24939047923188 | 0.23125618507833 |
| C1 | 2.16807116705866 | 26.26870706503977 | 0.23125618507833 |
| C1 | 15.17518087723365 | 3.73973218538307 | 0.23125618507833 |
| C1 | 15.17518087723365 | 18.75904877119096 | 0.23125618507833 |
| C1 | 10.83947763987874 | 11.24939047923188 | 6.36286650347188 |
| C1 | 10.83947763987874 | 26.26870706503977 | 6.36286650347188 |
| C1 | 23.84658735005374 | 3.73973218538307 | 6.36286650347188 |
| C1 | 23.84658735005374 | 18.75904877119096 | 6.36286650347188 |
| C1 | 6.50377440441356 | 3.73973218538307 | 12.49447682375516 |
| C1 | 6.50377440441356 | 18.75904877119096 | 12.49447682375516 |
| C1 | 19.51088411458856 | 11.24939047923188 | 12.49447682375516 |
| C1 | 19.51088411458856 | 26.26870706503977 | 12.49447682375516 |
| C1 | 2.16825431742496 | 11.24643082418998 | 18.85298421849575 |
| C1 | 2.16920150674032 | 26.27284136250260 | 18.84975975424224 |
| C1 | 15.17355024956793 | 3.74373550025900 | 18.85221228994013 |
| C1 | 15.17946803275301 | 18.76201733629153 | 18.84987591759687 |
| C1 | 2.16807116705866 | 3.73973218538307 | 0.23125618507833 |
| C1 | 2.16807116705866 | 18.75904877119096 | 0.23125618507833 |
| C1 | 15.17518087723365 | 11.24939047923188 | 0.23125618507833 |
| C1 | 15.17518087723365 | 26.26870706503977 | 0.23125618507833 |
| C1 | 10.83947763987874 | 3.73973218538307 | 6.36286650347188 |
| C1 | 10.83947763987874 | 18.75904877119096 | 6.36286650347188 |
| C1 | 23.84658735005374 | 11.24939047923188 | 6.36286650347188 |
| C1 | 23.84658735005374 | 26.26870706503977 | 6.36286650347188 |
| C1 | 6.50377440441356 | 11.24939047923188 | 12.49447682375516 |
| C1 | 6.50377440441356 | 26.26870706503977 | 12.49447682375516 |
| C1 | 19.51088411458856 | 3.73973218538307 | 12.49447682375516 |
| C1 | 19.51088411458856 | 18.75904877119096 | 12.49447682375516 |
| C1 | 2.16692598546800 | 3.73892033825278 | 18.85297950740852 |
| C1 | 2.17151342980698 | 18.75941904790734 | 18.84966181162690 |
| C1 | 15.17454235200410 | 11.24750589883112 | 18.85120595408679 |
| C1 | 15.17664490664419 | 26.27399975138914 | 18.85279003590832 |

Formamide adsorbed (100) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.09297732592380 | -0.03819235142316 | 5.51855138770084 |
| Na | -0.09297732592380 | 10.58206825561204 | 5.51855138770084 |
| Na | 10.52728328111139 | -0.03819235142316 | 5.51855138770084 |
| Na | 10.52728328111139 | 10.58206825561204 | 5.51855138770084 |
| Na | -0.09297732592380 | -0.03819235142316 | 16.13881199284631 |
| Na | -0.09297732592380 | 10.58206825561204 | 16.13881199284631 |
| Na | 10.52728328111139 | -0.03819235142316 | 16.13881199284631 |
| Na | 10.52728328111139 | 10.58206825561204 | 16.13881199284631 |
| Na | -0.09297732592380 | -0.03819235142316 | 26.75907259988151 |
| Na | -0.09297732592380 | 10.58206825561204 | 26.75907259988151 |
| Na | 10.52728328111139 | -0.03819235142316 | 26.75907259988151 |
| Na | 10.52728328111139 | 10.58206825561204 | 26.75907259988151 |
| Na | -0.11288377084435 | -0.05066111777465 | 36.95225870259642 |
| Na | -0.11025553030108 | 10.59507252499393 | 36.94924461021404 |
| Na | 10.54594099878800 | -0.01203994403003 | 36.93435645207116 |
| Na | 10.54761209682841 | 10.56230764274628 | 36.93606561486491 |
| Na | 5.21715297759380 | 5.27193795209444 | 5.51855138770084 |
| Na | 5.21715297759380 | 15.89219855912964 | 5.51855138770084 |
| Na | 15.83741358273927 | 5.27193795209444 | 5.51855138770084 |
| Na | 15.83741358273927 | 15.89219855912964 | 5.51855138770084 |
| Na | 5.21715297759380 | 5.27193795209444 | 16.13881199284631 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 5.21715297759380 | 15.89219855912964 | 16.13881199284631 |
| Na | 15.83741358273927 | 5.27193795209444 | 16.13881199284631 |
| Na | 15.83741358273927 | 15.89219855912964 | 16.13881199284631 |
| Na | 5.21715297759380 | 5.27193795209444 | 26.75907259988151 |
| Na | 5.21715297759380 | 15.89219855912964 | 26.75907259988151 |
| Na | 15.83741358273927 | 5.27193795209444 | 26.75907259988151 |
| Na | 15.83741358273927 | 15.89219855912964 | 26.75907259988151 |
| Na | 5.21376105525971 | 5.27205889456644 | 36.96867369519761 |
| Na | 5.17100513618717 | 15.89156705801209 | 36.91740148723729 |
| Na | 15.83976673585052 | 5.27548205218364 | 36.93099452158041 |
| Na | 15.90976768117468 | 15.89109891804887 | 37.16823774641657 |
| Na | -0.09297732592380 | 5.27193795209444 | 0.20842108418324 |
| Na | -0.09297732592380 | 15.89219855912964 | 0.20842108418324 |
| Na | 10.52728328111139 | 5.27193795209444 | 0.20842108418324 |
| Na | 10.52728328111139 | 15.89219855912964 | 0.20842108418324 |
| Na | -0.09297732592380 | 5.27193795209444 | 10.82868169121844 |
| Na | -0.09297732592380 | 15.89219855912964 | 10.82868169121844 |
| Na | 10.52728328111139 | 5.27193795209444 | 10.82868169121844 |
| Na | 10.52728328111139 | 15.89219855912964 | 10.82868169121844 |
| Na | -0.09297732592380 | 5.27193795209444 | 21.44894229636391 |
| Na | -0.09297732592380 | 15.89219855912964 | 21.44894229636391 |
| Na | 10.52728328111139 | 5.27193795209444 | 21.44894229636391 |
| Na | 10.52728328111139 | 15.89219855912964 | 21.44894229636391 |
| Na | -0.09134782642458 | 5.27194741395315 | 31.93024417747658 |
| Na | -0.10554424087077 | 15.89239923670575 | 31.92024623937188 |
| Na | 10.52966730478863 | 5.27297116363273 | 31.91794557907292 |
| Na | 10.52580117080129 | 15.89237476475244 | 31.87428011969861 |
| Na | 5.21715297759380 | -0.03819235142316 | 0.20842108418324 |
| Na | 5.21715297759380 | 10.58206825561204 | 0.20842108418324 |
| Na | 15.83741358273927 | -0.03819235142316 | 0.20842108418324 |
| Na | 15.83741358273927 | 10.58206825561204 | 0.20842108418324 |
| Na | 5.21715297759380 | -0.03819235142316 | 10.82868169121844 |
| Na | 5.21715297759380 | 10.58206825561204 | 10.82868169121844 |
| Na | 15.83741358273927 | -0.03819235142316 | 10.82868169121844 |
| Na | 15.83741358273927 | 10.58206825561204 | 10.82868169121844 |
| Na | 5.21715297759380 | -0.03819235142316 | 21.44894229636391 |
| Na | 5.21715297759380 | 10.58206825561204 | 21.44894229636391 |
| Na | 15.83741358273927 | -0.03819235142316 | 21.44894229636391 |
| Na | 15.83741358273927 | 10.58206825561204 | 21.44894229636391 |
| Na | 5.21750624299560 | -0.03939336686190 | 31.92453006897326 |
| Na | 5.21904490713945 | 10.58362326588687 | 31.92375482205856 |
| Na | 15.83872642650090 | -0.04413096316959 | 31.93264172025452 |
| Na | 15.83993244593442 | 10.58437798659639 | 31.92873757631590 |
| Cl | 5.21715297759380 | 5.27193795209444 | 0.20842108418324 |
| Cl | 5.21715297759380 | 15.89219855912964 | 0.20842108418324 |
| Cl | 15.83741358273927 | 5.27193795209444 | 0.20842108418324 |
| Cl | 15.83741358273927 | 15.89219855912964 | 0.20842108418324 |
| Cl | 5.21715297759380 | 5.27193795209444 | 10.82868169121844 |
| Cl | 5.21715297759380 | 15.89219855912964 | 10.82868169121844 |
| Cl | 15.83741358273927 | 5.27193795209444 | 10.82868169121844 |
| Cl | 15.83741358273927 | 15.89219855912964 | 10.82868169121844 |
| Cl | 5.21715297759380 | 5.27193795209444 | 21.44894229636391 |
| Cl | 5.21715297759380 | 15.89219855912964 | 21.44894229636391 |
| Cl | 15.83741358273927 | 5.27193795209444 | 21.44894229636391 |
| Cl | 15.83741358273927 | 15.89219855912964 | 21.44894229636391 |
| Cl | 5.22001668746087 | 5.27180553898486 | 31.89048252377991 |
| Cl | 5.21619825016093 | 15.89277949117608 | 31.85472531123595 |
| Cl | 15.83807809926194 | 5.26940510870541 | 31.86481575899338 |
| Cl | 15.82051345964727 | 15.89050043800563 | 31.94628853053397 |
| Cl | -0.09297732592380 | -0.03819235142316 | 0.20842108418324 |
| Cl | -0.09297732592380 | 10.58206825561204 | 0.20842108418324 |
| Cl | 10.52728328111139 | -0.03819235142316 | 0.20842108418324 |
| Cl | 10.52728328111139 | 10.58206825561204 | 0.20842108418324 |
| Cl | -0.09297732592380 | -0.03819235142316 | 10.82868169121844 |
| Cl | -0.09297732592380 | 10.58206825561204 | 10.82868169121844 |
| Cl | 10.52728328111139 | -0.03819235142316 | 10.82868169121844 |
| Cl | 10.52728328111139 | 10.58206825561204 | 10.82868169121844 |
| Cl | -0.09297732592380 | -0.03819235142316 | 21.44894229636391 |
| Cl | -0.09297732592380 | 10.58206825561204 | 21.44894229636391 |
| Cl | 10.52728328111139 | -0.03819235142316 | 21.44894229636391 |
| Cl | 10.52728328111139 | 10.58206825561204 | 21.44894229636391 |

| | | | |
|----|-------------------|--------------------|--------------------|
| C1 | -0.08771681594116 | -0.03436250773632 | 31.88382262435856 |
| C1 | -0.08606171443239 | 10.57843517776824 | 31.88172655147907 |
| C1 | 10.52284930898993 | -0.04083748233853 | 31.87693404161992 |
| C1 | 10.52342089256123 | 10.58543851034637 | 31.87624061795671 |
| C1 | 5.21715297759380 | -0.03819235142316 | 5.51855138770084 |
| C1 | 5.21715297759380 | 10.58206825561204 | 5.51855138770084 |
| C1 | 15.83741358273927 | -0.03819235142316 | 5.51855138770084 |
| C1 | 15.83741358273927 | 10.58206825561204 | 5.51855138770084 |
| C1 | 5.21715297759380 | -0.03819235142316 | 16.13881199284631 |
| C1 | 5.21715297759380 | 10.58206825561204 | 16.13881199284631 |
| C1 | 15.83741358273927 | -0.03819235142316 | 16.13881199284631 |
| C1 | 15.83741358273927 | 10.58206825561204 | 16.13881199284631 |
| C1 | 5.21715297759380 | -0.03819235142316 | 26.75907259988151 |
| C1 | 5.21715297759380 | 10.58206825561204 | 26.75907259988151 |
| C1 | 15.83741358273927 | -0.03819235142316 | 26.75907259988151 |
| C1 | 15.83741358273927 | 10.58206825561204 | 26.75907259988151 |
| C1 | 5.22532325006918 | -0.03043266163268 | 37.12372678955887 |
| C1 | 5.22475650041731 | 10.57328154313632 | 37.12242400669912 |
| C1 | 15.82104107874027 | 0.03924042565742 | 37.09349465054476 |
| C1 | 15.82760903353701 | 10.50843005425962 | 37.08193856333013 |
| C1 | -0.09297732592380 | 5.27193795209444 | 5.51855138770084 |
| C1 | -0.09297732592380 | 15.89219855912964 | 5.51855138770084 |
| C1 | 10.52728328111139 | 5.27193795209444 | 5.51855138770084 |
| C1 | 10.52728328111139 | 15.89219855912964 | 5.51855138770084 |
| C1 | -0.09297732592380 | 5.27193795209444 | 16.13881199284631 |
| C1 | -0.09297732592380 | 15.89219855912964 | 16.13881199284631 |
| C1 | 10.52728328111139 | 5.27193795209444 | 16.13881199284631 |
| C1 | 10.52728328111139 | 15.89219855912964 | 16.13881199284631 |
| C1 | -0.09297732592380 | 5.27193795209444 | 26.75907259988151 |
| C1 | -0.09297732592380 | 15.89219855912964 | 26.75907259988151 |
| C1 | 10.52728328111139 | 5.27193795209444 | 26.75907259988151 |
| C1 | 10.52728328111139 | 15.89219855912964 | 26.75907259988151 |
| C1 | -0.08021043637883 | 5.27172346439980 | 37.13125479514697 |
| C1 | -0.00734189591068 | 15.89276700764530 | 37.07468954745849 |
| C1 | 10.51198928349618 | 5.27602502341168 | 37.11529940661610 |
| C1 | 10.37160846307556 | 15.88816280710477 | 37.05398156764312 |
| C | 35.69967980374714 | -68.84312643570856 | 118.51757137686624 |
| N | 33.20254250072100 | -68.76817535657943 | 118.25624166504640 |
| O | 37.21588368899578 | -69.06939021569822 | 116.75558285398483 |
| H | 32.40119831706101 | -68.88808758957991 | 116.46114786355044 |
| H | 32.05547732933476 | -68.57073524036194 | 119.80695091565723 |
| H | 15.12372128403078 | 16.27263754231194 | 45.14605667330827 |

Formamide adsorbed (110) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.17726733140716 | 7.48982612461360 | 4.11318466777784 |
| Na | -0.17726733140716 | 22.50914271042150 | 4.11318466777784 |
| Na | 10.44299327373831 | 7.48982612461360 | 4.11318466777784 |
| Na | 10.44299327373831 | 22.50914271042150 | 4.11318466777784 |
| Na | -0.17726733140716 | -0.01983216734548 | 11.62284296162665 |
| Na | -0.17726733140716 | 14.99948441846241 | 11.62284296162665 |
| Na | 10.44299327373831 | -0.01983216734548 | 11.62284296162665 |
| Na | 10.44299327373831 | 14.99948441846241 | 11.62284296162665 |
| Na | -0.17726733140716 | 7.48982612461360 | 19.13250125358573 |
| Na | -0.17726733140716 | 22.50914271042150 | 19.13250125358573 |
| Na | 10.44299327373831 | 7.48982612461360 | 19.13250125358573 |
| Na | 10.44299327373831 | 22.50914271042150 | 19.13250125358573 |
| Na | -0.17090046425711 | -0.02687080945626 | 26.10911266022342 |
| Na | -0.22633839582572 | 15.00734100584968 | 26.08439937187106 |
| Na | 10.44663729687582 | -0.07906143943113 | 26.11585324150168 |
| Na | 10.37375064527250 | 15.31398831357233 | 26.24836395543434 |
| Na | 5.13286297211044 | 11.24465527153801 | 0.35835552274316 |
| Na | 5.13286297211044 | 26.26397185734590 | 0.35835552274316 |
| Na | 15.75312357725591 | 11.24465527153801 | 0.35835552274316 |
| Na | 15.75312357725591 | 26.26397185734590 | 0.35835552274316 |
| Na | 5.13286297211044 | 3.73499697957892 | 7.86801381470224 |
| Na | 5.13286297211044 | 18.75431356538682 | 7.86801381470224 |
| Na | 15.75312357725591 | 3.73499697957892 | 7.86801381470224 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 15.75312357725591 | 18.75431356538682 | 7.86801381470224 |
| Na | 5.13286297211044 | 11.24465527153801 | 15.37767210666132 |
| Na | 5.13286297211044 | 26.26397185734590 | 15.37767210666132 |
| Na | 15.75312357725591 | 11.24465527153801 | 15.37767210666132 |
| Na | 15.75312357725591 | 26.26397185734590 | 15.37767210666132 |
| Na | 5.13452363508319 | 3.73412965764852 | 22.82665902172672 |
| Na | 5.15043943952093 | 18.74488995662547 | 22.82546759664806 |
| Na | 15.75029023906711 | 3.74225121109467 | 22.82858722456534 |
| Na | 15.73422921106640 | 18.73556593076173 | 22.83705348484368 |
| Na | 5.13286297211044 | 3.73499697957892 | 0.35835552274316 |
| Na | 5.13286297211044 | 18.75431356538682 | 0.35835552274316 |
| Na | 15.75312357725591 | 3.73499697957892 | 0.35835552274316 |
| Na | 15.75312357725591 | 18.75431356538682 | 0.35835552274316 |
| Na | 5.13286297211044 | 11.24465527153801 | 7.86801381470224 |
| Na | 5.13286297211044 | 26.26397185734590 | 7.86801381470224 |
| Na | 15.75312357725591 | 11.24465527153801 | 7.86801381470224 |
| Na | 15.75312357725591 | 26.26397185734590 | 7.86801381470224 |
| Na | 5.13286297211044 | 3.73499697957892 | 15.37767210666132 |
| Na | 5.13286297211044 | 18.75431356538682 | 15.37767210666132 |
| Na | 15.75312357725591 | 3.73499697957892 | 15.37767210666132 |
| Na | 15.75312357725591 | 18.75431356538682 | 15.37767210666132 |
| Na | 5.13313218249420 | 11.27013064108315 | 22.84288095045835 |
| Na | 5.17092147801162 | 26.23445379670156 | 22.84202847421637 |
| Na | 15.72391267269592 | 11.28529471435809 | 22.85709582752878 |
| Na | 15.75428221180684 | 26.28740906844812 | 22.79723880732167 |
| Na | -0.17726733140716 | -0.01983216734548 | 4.11318466777784 |
| Na | -0.17726733140716 | 14.99948441846241 | 4.11318466777784 |
| Na | 10.44299327373831 | -0.01983216734548 | 4.11318466777784 |
| Na | 10.44299327373831 | 14.99948441846241 | 4.11318466777784 |
| Na | -0.17726733140716 | 7.48982612461360 | 11.62284296162665 |
| Na | -0.17726733140716 | 22.50914271042150 | 11.62284296162665 |
| Na | 10.44299327373831 | 7.48982612461360 | 11.62284296162665 |
| Na | 10.44299327373831 | 22.50914271042150 | 11.62284296162665 |
| Na | -0.17726733140716 | -0.01983216734548 | 19.13250125358573 |
| Na | -0.17726733140716 | 14.99948441846241 | 19.13250125358573 |
| Na | 10.44299327373831 | -0.01983216734548 | 19.13250125358573 |
| Na | 10.44299327373831 | 14.99948441846241 | 19.13250125358573 |
| Na | -0.18496077873806 | 7.49818825909273 | 26.10429287594710 |
| Na | -0.06912862884760 | 22.50377751339098 | 26.08300324976882 |
| Na | 10.43506638098029 | 7.53777082722399 | 26.11083544416308 |
| Na | 10.43792382829499 | 22.11367608652130 | 26.29071207349884 |
| Cl | 5.13286297211044 | -0.01983216734548 | 4.11318466777784 |
| Cl | 5.13286297211044 | 14.99948441846241 | 4.11318466777784 |
| Cl | 15.75312357725591 | -0.01983216734548 | 4.11318466777784 |
| Cl | 15.75312357725591 | 14.99948441846241 | 4.11318466777784 |
| Cl | 5.13286297211044 | 7.48982612461360 | 11.62284296162665 |
| Cl | 5.13286297211044 | 22.50914271042150 | 11.62284296162665 |
| Cl | 15.75312357725591 | 7.48982612461360 | 11.62284296162665 |
| Cl | 15.75312357725591 | 22.50914271042150 | 11.62284296162665 |
| Cl | 5.13286297211044 | -0.01983216734548 | 19.13250125358573 |
| Cl | 5.13286297211044 | 14.99948441846241 | 19.13250125358573 |
| Cl | 15.75312357725591 | -0.01983216734548 | 19.13250125358573 |
| Cl | 15.75312357725591 | 14.99948441846241 | 19.13250125358573 |
| Cl | 5.11849154634835 | 7.47960085245606 | 26.32708416134991 |
| Cl | 5.10333359200660 | 22.49464115055954 | 26.33743340710015 |
| Cl | 15.75318592687968 | 7.48540341903930 | 26.33076957326901 |
| Cl | 15.94640976175613 | 22.58445255594518 | 26.32795595437233 |
| Cl | -0.17726733140716 | 3.73499697957892 | 0.35835552274316 |
| Cl | -0.17726733140716 | 18.75431356538682 | 0.35835552274316 |
| Cl | 10.44299327373831 | 3.73499697957892 | 0.35835552274316 |
| Cl | 10.44299327373831 | 18.75431356538682 | 0.35835552274316 |
| Cl | -0.17726733140716 | 11.24465527153801 | 7.86801381470224 |
| Cl | -0.17726733140716 | 26.26397185734590 | 7.86801381470224 |
| Cl | 10.44299327373831 | 11.24465527153801 | 7.86801381470224 |
| Cl | 10.44299327373831 | 26.26397185734590 | 7.86801381470224 |
| Cl | -0.17726733140716 | 3.73499697957892 | 15.37767210666132 |
| Cl | -0.17726733140716 | 18.75431356538682 | 15.37767210666132 |
| Cl | 10.44299327373831 | 3.73499697957892 | 15.37767210666132 |
| Cl | 10.44299327373831 | 18.75431356538682 | 15.37767210666132 |
| Cl | -0.19097568439733 | 11.23066703499092 | 22.73539237415702 |
| Cl | -0.16227839605976 | 26.27542348050034 | 22.73887572711021 |

| | | | |
|----|--------------------|-------------------|-------------------|
| Cl | 10.42788397039565 | 11.32153524892497 | 22.82187120405753 |
| Cl | 10.47038299631931 | 26.15518631287211 | 22.84915692556124 |
| Cl | -0.17726733140716 | 11.24465527153801 | 0.35835552274316 |
| Cl | -0.17726733140716 | 26.26397185734590 | 0.35835552274316 |
| Cl | 10.44299327373831 | 11.24465527153801 | 0.35835552274316 |
| Cl | 10.44299327373831 | 26.26397185734590 | 0.35835552274316 |
| Cl | -0.17726733140716 | 3.73499697957892 | 7.86801381470224 |
| Cl | -0.17726733140716 | 18.75431356538682 | 7.86801381470224 |
| Cl | 10.44299327373831 | 3.73499697957892 | 7.86801381470224 |
| Cl | 10.44299327373831 | 18.75431356538682 | 7.86801381470224 |
| Cl | -0.17726733140716 | 11.24465527153801 | 15.37767210666132 |
| Cl | -0.17726733140716 | 26.26397185734590 | 15.37767210666132 |
| Cl | 10.44299327373831 | 11.24465527153801 | 15.37767210666132 |
| Cl | 10.44299327373831 | 26.26397185734590 | 15.37767210666132 |
| Cl | -0.17936627856008 | 3.73220623014781 | 22.75129038493356 |
| Cl | -0.18399999095350 | 18.76251226690203 | 22.72598639843014 |
| Cl | 10.44284035899000 | 3.72840067889031 | 22.77167008530595 |
| Cl | 10.44204576883869 | 18.75246489167217 | 22.53849380998324 |
| Cl | 5.13286297211044 | 7.48982612461360 | 4.11318466777784 |
| Cl | 5.13286297211044 | 22.50914271042150 | 4.11318466777784 |
| Cl | 15.75312357725591 | 7.48982612461360 | 4.11318466777784 |
| Cl | 15.75312357725591 | 22.50914271042150 | 4.11318466777784 |
| Cl | 5.13286297211044 | -0.01983216734548 | 11.62284296162665 |
| Cl | 5.13286297211044 | 14.99948441846241 | 11.62284296162665 |
| Cl | 15.75312357725591 | -0.01983216734548 | 11.62284296162665 |
| Cl | 15.75312357725591 | 14.99948441846241 | 11.62284296162665 |
| Cl | 5.13286297211044 | 7.48982612461360 | 19.13250125358573 |
| Cl | 5.13286297211044 | 22.50914271042150 | 19.13250125358573 |
| Cl | 15.75312357725591 | 7.48982612461360 | 19.13250125358573 |
| Cl | 15.75312357725591 | 22.50914271042150 | 19.13250125358573 |
| Cl | 5.12983784183777 | -0.01939631146338 | 26.32439627538095 |
| Cl | 4.99253443474252 | 14.99891653308514 | 26.33015216005973 |
| Cl | 15.76729198029176 | -0.01530153006355 | 26.32095783743830 |
| Cl | 15.80446915572276 | 15.01819564751370 | 26.36337577710367 |
| H | -73.44411997683102 | 17.16660870045162 | 96.89666489507866 |
| C | -72.82569926384291 | 18.39836357518365 | 95.31312949163002 |
| N | -70.62290644659787 | 19.50875940857883 | 95.64160094590378 |
| O | -74.18005855478158 | 18.67317210252018 | 93.39921311290149 |
| H | -69.85251381690831 | 20.58967617960769 | 94.16864126984056 |
| H | -69.58444091220869 | 19.16634128984301 | 97.24441330760345 |

Formamide adsorbed (111) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 0.00021954838120 | -0.01509695965161 | 3.29706134427511 |
| Na | 0.00021954838120 | 15.00421962426656 | 3.29706134427511 |
| Na | 13.00732925855620 | 7.49456133230747 | 3.29706134427511 |
| Na | 13.00732925855620 | 22.51387791811536 | 3.29706134427511 |
| Na | 8.67162602120129 | -0.01509695965161 | 9.42867166455839 |
| Na | 8.67162602120129 | 15.00421962426656 | 9.42867166455839 |
| Na | 21.67873573137628 | 7.49456133230747 | 9.42867166455839 |
| Na | 21.67873573137628 | 22.51387791811536 | 9.42867166455839 |
| Na | 4.33592278573611 | 7.49456133230747 | 15.56028198484167 |
| Na | 4.33592278573611 | 22.51387791811536 | 15.56028198484167 |
| Na | 17.34303249591110 | -0.01509695965161 | 15.56028198484167 |
| Na | 17.34303249591110 | 15.00421962426656 | 15.56028198484167 |
| Na | -0.05500044107342 | -0.05436023587734 | 21.47560441391555 |
| Na | -0.05703365788253 | 15.04325118416456 | 21.49819956683592 |
| Na | 13.02845858493648 | 7.49757804007081 | 21.49488450722224 |
| Na | 13.43011358568505 | 22.49777898598803 | 21.60564079604918 |
| Na | 0.00021954838120 | 7.49456133230747 | 3.29706134427511 |
| Na | 0.00021954838120 | 22.51387791811536 | 3.29706134427511 |
| Na | 13.00732925855620 | -0.01509695965161 | 3.29706134427511 |
| Na | 13.00732925855620 | 15.00421962426656 | 3.29706134427511 |
| Na | 8.67162602120129 | 7.49456133230747 | 9.42867166455839 |
| Na | 8.67162602120129 | 22.51387791811536 | 9.42867166455839 |
| Na | 21.67873573137628 | -0.01509695965161 | 9.42867166455839 |
| Na | 21.67873573137628 | 15.00421962426656 | 9.42867166455839 |
| Na | 4.33592278573611 | -0.01509695965161 | 15.56028198484167 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 4.33592278573611 | 15.00421962426656 | 15.56028198484167 |
| Na | 17.34303249591110 | 7.49456133230747 | 15.56028198484167 |
| Na | 17.34303249591110 | 22.51387791811536 | 15.56028198484167 |
| Na | -0.00481136554643 | 7.49653202752774 | 21.48502310560952 |
| Na | -0.01550166906772 | 22.51206776646777 | 21.39980379139940 |
| Na | 13.02518147480285 | -0.02707291755505 | 21.39642186949597 |
| Na | 13.02256591999105 | 15.02149036800509 | 21.41089257579948 |
| Na | 6.50377440441356 | 3.73973218538307 | 3.29706134427511 |
| Na | 6.50377440441356 | 18.75904877119096 | 3.29706134427511 |
| Na | 19.51088411458856 | 11.24939047923188 | 3.29706134427511 |
| Na | 19.51088411458856 | 26.26870706503977 | 3.29706134427511 |
| Na | 2.16807116705866 | 11.24939047923188 | 9.42867166455839 |
| Na | 2.16807116705866 | 26.26870706503977 | 9.42867166455839 |
| Na | 15.17518087723365 | 3.73973218538307 | 9.42867166455839 |
| Na | 15.17518087723365 | 18.75904877119096 | 9.42867166455839 |
| Na | 10.83947763987874 | 11.24939047923188 | 15.56028198484167 |
| Na | 10.83947763987874 | 26.26870706503977 | 15.56028198484167 |
| Na | 23.84658735005374 | 3.73973218538307 | 15.56028198484167 |
| Na | 23.84658735005374 | 18.75904877119096 | 15.56028198484167 |
| Na | 6.49727733702322 | 3.73072424833908 | 21.51597131098526 |
| Na | 6.57484412970113 | 18.80544517583371 | 21.48612413374926 |
| Na | 19.51793005860108 | 11.30991316491515 | 21.47270541719254 |
| Na | 19.29512687548260 | 25.92098891080969 | 21.63014257491528 |
| Na | 6.50377440441356 | 11.24939047923188 | 3.29706134427511 |
| Na | 6.50377440441356 | 26.26870706503977 | 3.29706134427511 |
| Na | 19.51088411458856 | 3.73973218538307 | 3.29706134427511 |
| Na | 19.51088411458856 | 18.75904877119096 | 3.29706134427511 |
| Na | 2.16807116705866 | 3.73973218538307 | 9.42867166455839 |
| Na | 2.16807116705866 | 18.75904877119096 | 9.42867166455839 |
| Na | 15.17518087723365 | 11.24939047923188 | 9.42867166455839 |
| Na | 15.17518087723365 | 26.26870706503977 | 9.42867166455839 |
| Na | 10.83947763987874 | 3.73973218538307 | 15.56028198484167 |
| Na | 10.83947763987874 | 18.75904877119096 | 15.56028198484167 |
| Na | 23.84658735005374 | 11.24939047923188 | 15.56028198484167 |
| Na | 23.84658735005374 | 26.26870706503977 | 15.56028198484167 |
| Na | 6.49591279224453 | 11.26076760182357 | 21.51668474873786 |
| Na | 6.57692605420112 | 26.22943159252164 | 21.49805889184372 |
| Na | 19.52592149306517 | 3.67461529958992 | 21.47531530282596 |
| Na | 19.29743245284893 | 19.09046035963573 | 21.61483590290695 |
| Cl | 8.67162602120129 | -0.01509695965161 | 0.23125618507833 |
| Cl | 8.67162602120129 | 15.00421962426656 | 0.23125618507833 |
| Cl | 21.67873573137628 | 7.49456133230747 | 0.23125618507833 |
| Cl | 21.67873573137628 | 22.51387791811536 | 0.23125618507833 |
| Cl | 4.33592278573611 | 7.49456133230747 | 6.36286650347188 |
| Cl | 4.33592278573611 | 22.51387791811536 | 6.36286650347188 |
| Cl | 17.34303249591110 | -0.01509695965161 | 6.36286650347188 |
| Cl | 17.34303249591110 | 15.00421962426656 | 6.36286650347188 |
| Cl | 0.00021954838120 | -0.01509695965161 | 12.49447682375516 |
| Cl | 0.00021954838120 | 15.00421962426656 | 12.49447682375516 |
| Cl | 13.00732925855620 | 7.49456133230747 | 12.49447682375516 |
| Cl | 13.00732925855620 | 22.51387791811536 | 12.49447682375516 |
| Cl | 8.66138890613012 | -0.01256238149400 | 18.85365069277469 |
| Cl | 8.66003252307856 | 15.00436480247611 | 18.84788865892711 |
| Cl | 21.66219339391098 | 7.49651246319317 | 18.86256915506612 |
| Cl | 21.70489299158610 | 22.51414137050363 | 18.75513283536132 |
| Cl | 8.67162602120129 | 7.49456133230747 | 0.23125618507833 |
| Cl | 8.67162602120129 | 22.51387791811536 | 0.23125618507833 |
| Cl | 21.67873573137628 | -0.01509695965161 | 0.23125618507833 |
| Cl | 21.67873573137628 | 15.00421962426656 | 0.23125618507833 |
| Cl | 4.33592278573611 | -0.01509695965161 | 6.36286650347188 |
| Cl | 4.33592278573611 | 15.00421962426656 | 6.36286650347188 |
| Cl | 17.34303249591110 | 7.49456133230747 | 6.36286650347188 |
| Cl | 17.34303249591110 | 22.51387791811536 | 6.36286650347188 |
| Cl | 0.00021954838120 | 7.49456133230747 | 12.49447682375516 |
| Cl | 0.00021954838120 | 22.51387791811536 | 12.49447682375516 |
| Cl | 13.00732925855620 | -0.01509695965161 | 12.49447682375516 |
| Cl | 13.00732925855620 | 15.00421962426656 | 12.49447682375516 |
| Cl | 8.66760712553346 | 7.49750936931315 | 18.86966690781008 |
| Cl | 8.86737057120450 | 22.51419052794932 | 18.92132990357415 |
| Cl | 21.57555168851576 | -0.18247599297411 | 18.93173866813843 |
| Cl | 21.58351258878513 | 15.16200040411869 | 18.92419576583928 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Cl | 2.16807116705866 | 11.24939047923188 | 0.23125618507833 |
| Cl | 2.16807116705866 | 26.26870706503977 | 0.23125618507833 |
| Cl | 15.17518087723365 | 3.73973218538307 | 0.23125618507833 |
| Cl | 15.17518087723365 | 18.75904877119096 | 0.23125618507833 |
| Cl | 10.83947763987874 | 11.24939047923188 | 6.36286650347188 |
| Cl | 10.83947763987874 | 26.26870706503977 | 6.36286650347188 |
| Cl | 23.84658735005374 | 3.73973218538307 | 6.36286650347188 |
| Cl | 23.84658735005374 | 18.75904877119096 | 6.36286650347188 |
| Cl | 6.50377440441356 | 3.73973218538307 | 12.49447682375516 |
| Cl | 6.50377440441356 | 18.75904877119096 | 12.49447682375516 |
| Cl | 19.51088411458856 | 11.24939047923188 | 12.49447682375516 |
| Cl | 19.51088411458856 | 26.26870706503977 | 12.49447682375516 |
| Cl | 2.15051667338355 | 11.26862666097260 | 18.86419647760085 |
| Cl | 2.20271059715106 | 26.26968701464723 | 18.84725915902953 |
| Cl | 15.17391015735706 | 3.75427249596894 | 18.83051974580610 |
| Cl | 15.15833376284918 | 18.69750459972000 | 18.76717389621949 |
| Cl | 2.16807116705866 | 3.73973218538307 | 0.23125618507833 |
| Cl | 2.16807116705866 | 18.75904877119096 | 0.23125618507833 |
| Cl | 15.17518087723365 | 11.24939047923188 | 0.23125618507833 |
| Cl | 15.17518087723365 | 26.26870706503977 | 0.23125618507833 |
| Cl | 10.83947763987874 | 3.73973218538307 | 6.36286650347188 |
| Cl | 10.83947763987874 | 18.75904877119096 | 6.36286650347188 |
| Cl | 23.84658735005374 | 11.24939047923188 | 6.36286650347188 |
| Cl | 23.84658735005374 | 26.26870706503977 | 6.36286650347188 |
| Cl | 6.50377440441356 | 11.24939047923188 | 12.49447682375516 |
| Cl | 6.50377440441356 | 26.26870706503977 | 12.49447682375516 |
| Cl | 19.51088411458856 | 3.73973218538307 | 12.49447682375516 |
| Cl | 19.51088411458856 | 18.75904877119096 | 12.49447682375516 |
| Cl | 2.15097748876830 | 3.72379728337311 | 18.86385726420250 |
| Cl | 2.20332125080999 | 18.75735415739864 | 18.86002006192214 |
| Cl | 15.17212369153672 | 11.23752123038326 | 18.83693848404856 |
| Cl | 15.16032057743330 | 26.33824380481050 | 18.77524710291247 |
| H | 71.65277955314397 | 82.24904802533118 | 26.74686016165079 |
| C | 69.71745589388861 | 82.51101968089515 | 26.00917035371319 |
| N | 67.96831764849689 | 82.74893327095634 | 27.72411301276695 |
| O | 69.32296004497555 | 82.56434859496032 | 23.63172131901641 |
| H | 66.08345981515953 | 82.98944653268126 | 27.29562984612186 |
| H | 68.44207566543982 | 82.66355713971348 | 29.61157777242663 |

Citric acid adsorbed (100) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.09297732592380 | -0.03819235142316 | 5.51855138770084 |
| Na | -0.09297732592380 | 10.58206825561204 | 5.51855138770084 |
| Na | 10.52728328111139 | -0.03819235142316 | 5.51855138770084 |
| Na | -0.52728328111139 | 10.58206825561204 | 5.51855138770084 |
| Na | -0.09297732592380 | -0.03819235142316 | 16.13881199284631 |
| Na | -0.09297732592380 | 10.58206825561204 | 16.13881199284631 |
| Na | 10.52728328111139 | -0.03819235142316 | 16.13881199284631 |
| Na | 10.52728328111139 | 10.58206825561204 | 16.13881199284631 |
| Na | -0.09297732592380 | -0.03819235142316 | 26.75907259988151 |
| Na | -0.09297732592380 | 10.58206825561204 | 26.75907259988151 |
| Na | 10.52728328111139 | -0.03819235142316 | 26.75907259988151 |
| Na | 10.52728328111139 | 10.58206825561204 | 26.75907259988151 |
| Na | -0.07740318585919 | -0.00459979747866 | 36.93236716950472 |
| Na | -0.16496360617652 | 10.60787855643613 | 36.87778336957816 |
| Na | 10.53475348753624 | -0.08270115399308 | 36.87650900253016 |
| Na | 10.28977902084668 | 10.40730942225224 | 37.17023478441902 |
| Na | 5.21715297759380 | 5.27193795209444 | 5.51855138770084 |
| Na | 5.21715297759380 | 15.89219855912964 | 5.51855138770084 |
| Na | 15.83741358273927 | 5.27193795209444 | 5.51855138770084 |
| Na | 15.83741358273927 | 15.89219855912964 | 5.51855138770084 |
| Na | 5.21715297759380 | 5.27193795209444 | 16.13881199284631 |
| Na | 5.21715297759380 | 15.89219855912964 | 16.13881199284631 |
| Na | 15.83741358273927 | 5.27193795209444 | 16.13881199284631 |
| Na | 15.83741358273927 | 15.89219855912964 | 16.13881199284631 |
| Na | 5.21715297759380 | 5.27193795209444 | 26.75907259988151 |
| Na | 5.21715297759380 | 15.89219855912964 | 26.75907259988151 |
| Na | 15.83741358273927 | 5.27193795209444 | 26.75907259988151 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 15.83741358273927 | 15.89219855912964 | 26.75907259988151 |
| Na | 5.43068122993327 | 5.51832617203099 | 37.15091547362606 |
| Na | 5.19434405318499 | 15.95871799965275 | 36.90629767195561 |
| Na | 15.87273548931144 | 5.25614785601799 | 36.87711917997811 |
| Na | 15.79677597484325 | 15.85675607480261 | 36.89689581772141 |
| Na | -0.09297732592380 | 5.27193795209444 | 0.20842108418324 |
| Na | -0.09297732592380 | 15.89219855912964 | 0.20842108418324 |
| Na | 10.52728328111139 | 5.27193795209444 | 0.20842108418324 |
| Na | 10.52728328111139 | 15.89219855912964 | 0.20842108418324 |
| Na | -0.09297732592380 | 5.27193795209444 | 10.82868169121844 |
| Na | -0.09297732592380 | 15.89219855912964 | 10.82868169121844 |
| Na | 10.52728328111139 | 5.27193795209444 | 10.82868169121844 |
| Na | 10.52728328111139 | 15.89219855912964 | 10.82868169121844 |
| Na | -0.09297732592380 | 5.27193795209444 | 21.44894229636391 |
| Na | -0.09297732592380 | 15.89219855912964 | 21.44894229636391 |
| Na | 10.52728328111139 | 5.27193795209444 | 21.44894229636391 |
| Na | 10.52728328111139 | 15.89219855912964 | 21.44894229636391 |
| Na | -0.03526310207461 | 5.28095367669979 | 31.95115115679127 |
| Na | -0.10216205629541 | 15.89483557934048 | 31.93747103064024 |
| Na | 10.56336450987621 | 5.22889312035355 | 31.87125342851215 |
| Na | 10.49768830105486 | 15.82639661360111 | 31.96237384151540 |
| Na | 5.21715297759380 | -0.03819235142316 | 0.20842108418324 |
| Na | 5.21715297759380 | 10.58206825561204 | 0.20842108418324 |
| Na | 15.83741358273927 | -0.03819235142316 | 0.20842108418324 |
| Na | 15.83741358273927 | 10.58206825561204 | 0.20842108418324 |
| Na | 5.21715297759380 | -0.03819235142316 | 10.82868169121844 |
| Na | 5.21715297759380 | 10.58206825561204 | 10.82868169121844 |
| Na | 15.83741358273927 | -0.03819235142316 | 10.82868169121844 |
| Na | 15.83741358273927 | 10.58206825561204 | 10.82868169121844 |
| Na | 5.21715297759380 | -0.03819235142316 | 21.44894229636391 |
| Na | 5.21715297759380 | 10.58206825561204 | 21.44894229636391 |
| Na | 15.83741358273927 | -0.03819235142316 | 21.44894229636391 |
| Na | 15.83741358273927 | 10.58206825561204 | 21.44894229636391 |
| Na | 5.21314255356818 | 0.03217543509529 | 31.95792167133135 |
| Na | 5.15307527298377 | 10.63833912365449 | 31.87462828095015 |
| Na | 15.82464615840180 | -0.04304517567105 | 31.93196758502586 |
| Na | 15.74604081570929 | 10.56236783052336 | 31.95400448261329 |
| Cl | 5.21715297759380 | 5.27193795209444 | 0.20842108418324 |
| Cl | 5.21715297759380 | 15.89219855912964 | 0.20842108418324 |
| Cl | 15.83741358273927 | 5.27193795209444 | 0.20842108418324 |
| Cl | 15.83741358273927 | 15.89219855912964 | 0.20842108418324 |
| Cl | 5.21715297759380 | 5.27193795209444 | 10.82868169121844 |
| Cl | 5.21715297759380 | 15.89219855912964 | 10.82868169121844 |
| Cl | 15.83741358273927 | 5.27193795209444 | 10.82868169121844 |
| Cl | 15.83741358273927 | 15.89219855912964 | 10.82868169121844 |
| Cl | 5.21715297759380 | 5.27193795209444 | 21.44894229636391 |
| Cl | 5.21715297759380 | 15.89219855912964 | 21.44894229636391 |
| Cl | 15.83741358273927 | 5.27193795209444 | 21.44894229636391 |
| Cl | 15.83741358273927 | 15.89219855912964 | 21.44894229636391 |
| Cl | 5.22674321295621 | 5.29689909314591 | 31.91933076721980 |
| Cl | 5.19135384505111 | 15.98648490589913 | 31.84986425345133 |
| Cl | 15.91321955695980 | 5.25309595021585 | 31.84064763206164 |
| Cl | 15.82223531006222 | 15.88647233559212 | 31.87458470764516 |
| Cl | -0.09297732592380 | -0.03819235142316 | 0.20842108418324 |
| Cl | -0.09297732592380 | 10.58206825561204 | 0.20842108418324 |
| Cl | 10.52728328111139 | -0.03819235142316 | 0.20842108418324 |
| Cl | 10.52728328111139 | 10.58206825561204 | 0.20842108418324 |
| Cl | -0.09297732592380 | -0.03819235142316 | 10.82868169121844 |
| Cl | -0.09297732592380 | 10.58206825561204 | 10.82868169121844 |
| Cl | 10.52728328111139 | -0.03819235142316 | 10.82868169121844 |
| Cl | 10.52728328111139 | 10.58206825561204 | 10.82868169121844 |
| Cl | -0.09297732592380 | -0.03819235142316 | 21.44894229636391 |
| Cl | -0.09297732592380 | 10.58206825561204 | 21.44894229636391 |
| Cl | 10.52728328111139 | -0.03819235142316 | 21.44894229636391 |
| Cl | 10.52728328111139 | 10.58206825561204 | 21.44894229636391 |
| Cl | -0.10852916910987 | -0.04219666785394 | 31.89450620045484 |
| Cl | -0.20054437121274 | 10.59860171514400 | 31.84309368410919 |
| Cl | 10.52925953023675 | -0.12819001577458 | 31.84052145693800 |
| Cl | 10.48976178813179 | 10.56861838692015 | 31.92731797247683 |
| Cl | 5.21715297759380 | -0.03819235142316 | 5.51855138770084 |
| Cl | 5.21715297759380 | 10.58206825561204 | 5.51855138770084 |

| | | | |
|----|-------------------|-------------------|-------------------|
| C1 | 15.83741358273927 | -0.03819235142316 | 5.51855138770084 |
| C1 | 15.83741358273927 | 10.58206825561204 | 5.51855138770084 |
| C1 | 5.21715297759380 | -0.03819235142316 | 16.13881199284631 |
| C1 | 5.21715297759380 | 10.58206825561204 | 16.13881199284631 |
| C1 | 15.83741358273927 | -0.03819235142316 | 16.13881199284631 |
| C1 | 15.83741358273927 | 10.58206825561204 | 16.13881199284631 |
| C1 | 5.21715297759380 | -0.03819235142316 | 26.75907259988151 |
| C1 | 5.21715297759380 | 10.58206825561204 | 26.75907259988151 |
| C1 | 15.83741358273927 | -0.03819235142316 | 26.75907259988151 |
| C1 | 15.83741358273927 | 10.58206825561204 | 26.75907259988151 |
| C1 | 5.20502325834474 | -0.02815202109229 | 37.19259559996154 |
| C1 | 4.93765543691852 | 10.86960416587917 | 36.87484051042208 |
| C1 | 15.87683398969228 | -0.09186101367916 | 37.17414278906811 |
| C1 | 15.80873138575453 | 10.57954625925097 | 37.18703765464573 |
| C1 | -0.09297732592380 | 5.27193795209444 | 5.51855138770084 |
| C1 | -0.09297732592380 | 15.89219855912964 | 5.51855138770084 |
| C1 | 10.52728328111139 | 5.27193795209444 | 5.51855138770084 |
| C1 | 10.52728328111139 | 15.89219855912964 | 5.51855138770084 |
| C1 | -0.09297732592380 | 5.27193795209444 | 16.13881199284631 |
| C1 | -0.09297732592380 | 15.89219855912964 | 16.13881199284631 |
| C1 | 10.52728328111139 | 5.27193795209444 | 16.13881199284631 |
| C1 | 10.52728328111139 | 15.89219855912964 | 16.13881199284631 |
| C1 | -0.09297732592380 | 5.27193795209444 | 26.75907259988151 |
| C1 | -0.09297732592380 | 15.89219855912964 | 26.75907259988151 |
| C1 | 10.52728328111139 | 5.27193795209444 | 26.75907259988151 |
| C1 | 10.52728328111139 | 15.89219855912964 | 26.75907259988151 |
| C1 | -0.09888313958361 | 5.27609201231309 | 37.17511808994931 |
| C1 | -0.16950408515211 | 15.95126252175333 | 37.18804297949559 |
| C1 | 10.77646322368802 | 5.02202002422286 | 36.85725276512606 |
| C1 | 10.51327945999295 | 15.89919780800961 | 37.20983305617438 |
| C | 8.72975740209257 | 10.21434122763625 | 46.35484283028010 |
| C | 9.19881902253679 | 9.60309802706266 | 49.10440679544094 |
| O | 11.26639780837667 | 9.52388498435315 | 50.09419248218313 |
| O | 7.06620886101091 | 8.94530384791846 | 50.28946763366552 |
| O | 10.91646527874250 | 11.24210158258009 | 45.30461507924029 |
| C | 8.08577371941505 | 7.69085869712211 | 45.09876632238374 |
| C | 7.93396528481041 | 7.85849853154712 | 42.24070215572480 |
| O | 6.41302263162388 | 6.43620222392238 | 41.15111729599827 |
| O | 9.45251452993977 | 9.41196289891326 | 41.19487627791850 |
| C | 6.51775344366360 | 12.03171983800025 | 46.00174802916890 |
| C | 7.09753430296436 | 14.60009509162332 | 46.96935724504181 |
| O | 6.80069866304227 | 16.55734414139665 | 45.80201094517731 |
| O | 8.00245504827775 | 14.53479356635968 | 49.33120556256577 |
| H | 7.53693792476522 | 8.40030868351219 | 52.02349394710555 |
| H | 10.68670874630189 | 10.76103285398699 | 43.40356604411809 |
| H | 9.60414438164615 | 6.32062794416921 | 45.54799291632685 |
| H | 6.30969331984695 | 6.91720789991359 | 45.86150198023606 |
| H | 6.09733175229170 | 12.17813570856064 | 43.96267747023697 |
| H | 4.80819738089900 | 11.31259538737491 | 46.96348341688640 |
| H | 8.38544296586704 | 16.30057246410808 | 49.84144489541952 |

Citric acid adsorbed (110) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.17726733140716 | 7.48982612461360 | 4.11318466777784 |
| Na | -0.17726733140716 | 22.50914271042150 | 4.11318466777784 |
| Na | 10.44299327373831 | 7.48982612461360 | 4.11318466777784 |
| Na | 10.44299327373831 | 22.50914271042150 | 4.11318466777784 |
| Na | -0.17726733140716 | -0.01983216734548 | 11.62284296162665 |
| Na | -0.17726733140716 | 14.99948441846241 | 11.62284296162665 |
| Na | 10.44299327373831 | -0.01983216734548 | 11.62284296162665 |
| Na | 10.44299327373831 | 14.99948441846241 | 11.62284296162665 |
| Na | -0.17726733140716 | 7.48982612461360 | 19.13250125358573 |
| Na | -0.17726733140716 | 22.50914271042150 | 19.13250125358573 |
| Na | 10.44299327373831 | 7.48982612461360 | 19.13250125358573 |
| Na | 10.44299327373831 | 22.50914271042150 | 19.13250125358573 |
| Na | -0.17110336415115 | -0.03530436613428 | 26.09516936325331 |
| Na | -0.24438262336448 | 15.01507773735747 | 26.06255740898206 |
| Na | 10.45029985255744 | -0.06118254403105 | 26.10310790617289 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 10.39593581077169 | 15.21821859793513 | 26.23394095337713 |
| Na | 5.13286297211044 | 11.24465527153801 | 0.35835552274316 |
| Na | 5.13286297211044 | 26.26397185734590 | 0.35835552274316 |
| Na | 15.75312357725591 | 11.24465527153801 | 0.35835552274316 |
| Na | 15.75312357725591 | 26.26397185734590 | 0.35835552274316 |
| Na | 5.13286297211044 | 3.73499697957892 | 7.86801381470224 |
| Na | 5.13286297211044 | 18.75431356538682 | 7.86801381470224 |
| Na | 15.75312357725591 | 3.73499697957892 | 7.86801381470224 |
| Na | 15.75312357725591 | 18.75431356538682 | 7.86801381470224 |
| Na | 5.13286297211044 | 11.24465527153801 | 15.37767210666132 |
| Na | 5.13286297211044 | 26.26397185734590 | 15.37767210666132 |
| Na | 15.75312357725591 | 11.24465527153801 | 15.37767210666132 |
| Na | 15.75312357725591 | 26.26397185734590 | 15.37767210666132 |
| Na | 5.13373611061786 | 3.73473319270914 | 22.83524491300712 |
| Na | 5.12648313765971 | 18.75042684283335 | 22.85643053999785 |
| Na | 15.75168876679071 | 3.74223986706874 | 22.83300872638410 |
| Na | 15.74841913052390 | 18.75908489897502 | 22.87290285744104 |
| Na | 5.13286297211044 | 3.73499697957892 | 0.35835552274316 |
| Na | 5.13286297211044 | 18.75431356538682 | 0.35835552274316 |
| Na | 15.75312357725591 | 3.73499697957892 | 0.35835552274316 |
| Na | 15.75312357725591 | 18.75431356538682 | 0.35835552274316 |
| Na | 5.13286297211044 | 11.24465527153801 | 7.86801381470224 |
| Na | 5.13286297211044 | 26.26397185734590 | 7.86801381470224 |
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| Na | 15.76152055072588 | 26.23179100062636 | 22.85680737973307 |
| Na | -0.17726733140716 | -0.01983216734548 | 4.11318466777784 |
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| C1 | 10.44299327373831 | 26.26397185734590 | 7.86801381470224 |
| C1 | -0.17726733140716 | 3.73499697957892 | 15.37767210666132 |
| C1 | -0.17726733140716 | 18.75431356538682 | 15.37767210666132 |
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| C1 | -0.20170622018782 | 11.21162580873560 | 22.71985715111222 |
| C1 | -0.18083244903032 | 26.30709795486907 | 22.70524224925674 |
| C1 | 10.42849387383331 | 11.29283014468015 | 22.80062125078951 |
| C1 | 10.45522406309943 | 26.21245205935841 | 22.80242227883937 |
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| C1 | 5.13286297211044 | 7.48982612461360 | 19.13250125358573 |
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| C1 | 5.13876317706310 | -0.00702686533757 | 26.34635312983890 |
| C1 | 4.90642302051304 | 14.96486348311959 | 26.30092325207894 |
| C1 | 15.76233769097904 | -0.00358788504352 | 26.34676623152873 |
| C1 | 15.87357414409653 | 15.01182712307383 | 26.36115442294100 |
| C | 11.65122053476004 | -13.41351188625298 | 35.26492000059500 |
| C | 11.07831741116997 | -13.30721767922361 | 38.06159030081951 |
| O | 9.74432633106883 | -14.79905244626986 | 39.17954957405735 |
| O | 12.06484062559710 | -11.25686483927474 | 39.15505497426081 |
| O | 10.97305907263382 | -15.78781084198572 | 34.34276211843248 |
| C | 10.03898198482284 | -11.33602336527528 | 34.04216634682032 |
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| O | 10.06365306047303 | -9.42456376090034 | 29.98981517554043 |
| O | 10.23362750601655 | -13.64838911728887 | 30.20551179790148 |
| C | 14.42867317444956 | -12.87055761661307 | 34.69662882164313 |
| C | 16.13512603668608 | -14.92327282019832 | 35.56956275109495 |
| O | 17.77101661234275 | -15.92474966799912 | 34.30498414993347 |
| O | 15.70970791132943 | -15.55798262089483 | 37.98137714890424 |
| H | 11.49080174826002 | -11.24287410828917 | 40.94432023299821 |
| H | 10.62166311830146 | -15.37057909146075 | 32.45026579666911 |
| H | 8.04482539708038 | -11.60349062786965 | 34.62107524680275 |
| H | 10.64176939042138 | -9.44780379041977 | 34.68570421286933 |
| H | 14.66723909041020 | -12.67467509770547 | 32.63274348283783 |
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| H | 16.92286069436307 | -16.92090358816336 | 38.42896594367098 |

Citric acid adsorbed (111) surface of NaCl:

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| Na | 0.00021954838120 | -0.01509695965161 | 3.29706134427511 |
| Na | 0.00021954838120 | 15.00421962426656 | 3.29706134427511 |
| Na | 13.00732925855620 | 7.49456133230747 | 3.29706134427511 |

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| Na | 8.67162602120129 | 15.00421962426656 | 9.42867166455839 |
| Na | 21.67873573137628 | 7.49456133230747 | 9.42867166455839 |
| Na | 21.67873573137628 | 22.51387791811536 | 9.42867166455839 |
| Na | 4.33592278573611 | 7.49456133230747 | 15.56028198484167 |
| Na | 4.33592278573611 | 22.51387791811536 | 15.56028198484167 |
| Na | 17.34303249591110 | -0.01509695965161 | 15.56028198484167 |
| Na | 17.34303249591110 | 15.00421962426656 | 15.56028198484167 |
| Na | 0.00165640919925 | -0.01793455350364 | 21.50490908479614 |
| Na | 0.34916573924389 | 14.97999640047991 | 21.33573423906788 |
| Na | 12.79321976992438 | 7.84825309979127 | 21.75564638657716 |
| Na | 13.00807828363118 | 22.45573555035640 | 21.46520429484829 |
| Na | 0.00021954838120 | 7.49456133230747 | 3.29706134427511 |
| Na | 0.00021954838120 | 22.51387791811536 | 3.29706134427511 |
| Na | 13.00732925855620 | -0.01509695965161 | 3.29706134427511 |
| Na | 13.00732925855620 | 15.00421962426656 | 3.29706134427511 |
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| Na | 8.67162602120129 | 22.51387791811536 | 9.42867166455839 |
| Na | 21.67873573137628 | -0.01509695965161 | 9.42867166455839 |
| Na | 21.67873573137628 | 15.00421962426656 | 9.42867166455839 |
| Na | 4.33592278573611 | -0.01509695965161 | 15.56028198484167 |
| Na | 4.33592278573611 | 15.00421962426656 | 15.56028198484167 |
| Na | 17.34303249591110 | 7.49456133230747 | 15.56028198484167 |
| Na | 17.34303249591110 | 22.51387791811536 | 15.56028198484167 |
| Na | 0.11669948315922 | 7.51230239297372 | 21.41263410015313 |
| Na | 0.07461034639098 | 22.48115087763337 | 21.37769744070770 |
| Na | 12.99139660154088 | 0.08144134539514 | 21.48346056855554 |
| Na | 13.05497107775300 | 14.72223924424525 | 21.41721424259036 |
| Na | 6.50377440441356 | 3.73973218538307 | 3.29706134427511 |
| Na | 6.50377440441356 | 18.75904877119096 | 3.29706134427511 |
| Na | 19.51088411458856 | 11.24939047923188 | 3.29706134427511 |
| Na | 19.51088411458856 | 26.26870706503977 | 3.29706134427511 |
| Na | 2.16807116705866 | 11.24939047923188 | 9.42867166455839 |
| Na | 2.16807116705866 | 26.26870706503977 | 9.42867166455839 |
| Na | 15.17518087723365 | 3.73973218538307 | 9.42867166455839 |
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| Na | 10.83947763987874 | 11.24939047923188 | 15.56028198484167 |
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| Na | 6.54236076373378 | 18.25184693119819 | 22.35041811819459 |
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| Na | 2.16807116705866 | 18.75904877119096 | 9.42867166455839 |
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| Na | 19.61378053168422 | 18.71644212725420 | 21.51293301310095 |
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| Cl | 4.33592278573611 | 7.49456133230747 | 6.36286650347188 |
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| C1 | 8.72088224665475 | 15.24777523544859 | 18.7036929980123 |
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| C1 | 21.63937291004747 | 0.00879958906953 | 18.88027477769834 |
| C1 | 21.87242437273907 | 15.01643002915197 | 18.86898286285763 |
| C1 | 2.16807116705866 | 11.24939047923188 | 0.23125618507833 |
| C1 | 2.16807116705866 | 26.26870706503977 | 0.23125618507833 |
| C1 | 15.17518087723365 | 3.73973218538307 | 0.23125618507833 |
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| O | 8.83485653309241 | -14.22808313611528 | 25.60284456981381 |
| C | 10.38145781390479 | -17.77023979884509 | 28.01357174204298 |
| C | 10.89342453407104 | -19.29047248570592 | 25.66387761572139 |
| O | 11.64929407046944 | -21.49147401832898 | 25.78485898395381 |
| O | 10.55349771120567 | -18.14396936044322 | 23.48357794020105 |
| C | 5.75110260209263 | -17.20790729108246 | 27.23792585513964 |
| C | 3.98942497506357 | -15.45789197466325 | 26.01566074848059 |
| O | 3.87002773211639 | -15.19251430507748 | 23.64761510247561 |
| O | 2.76439799587832 | -14.00170134650855 | 27.61044904203573 |
| H | 7.17817888124369 | -14.48429355529609 | 33.50417220007767 |
| H | 9.59124814601710 | -15.54655317367647 | 24.41020612824924 |
| H | 12.15915230981447 | -16.77164638209322 | 28.50280947321551 |
| H | 9.96865967834305 | -19.07694361920545 | 29.58560042359254 |

| | | | |
|---|------------------|--------------------|-------------------|
| H | 6.06952841212564 | -18.88066274036153 | 26.03227595756472 |
| H | 5.01288557190453 | -17.91104244204161 | 29.05618935243838 |
| H | 1.75016320260631 | -12.68885714645367 | 26.73180082833605 |

NTA adsorbed (100) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.09297732592380 | -0.03819235142316 | 5.51855138770084 |
| Na | -0.09297732592380 | 10.58206825561204 | 5.51855138770084 |
| Na | 10.52728328111139 | -0.03819235142316 | 5.51855138770084 |
| Na | 10.52728328111139 | 10.58206825561204 | 5.51855138770084 |
| Na | -0.09297732592380 | -0.03819235142316 | 16.13881199284631 |
| Na | -0.09297732592380 | 10.58206825561204 | 16.13881199284631 |
| Na | 10.52728328111139 | -0.03819235142316 | 16.13881199284631 |
| Na | 10.52728328111139 | 10.58206825561204 | 16.13881199284631 |
| Na | -0.09297732592380 | -0.03819235142316 | 26.75907259988151 |
| Na | -0.09297732592380 | 10.58206825561204 | 26.75907259988151 |
| Na | 10.52728328111139 | -0.03819235142316 | 26.75907259988151 |
| Na | 10.52728328111139 | 10.58206825561204 | 26.75907259988151 |
| Na | -0.08974554276100 | -0.10912279633641 | 36.78571692188223 |
| Na | 0.07253647968319 | 10.61272213614381 | 36.79331142882240 |
| Na | 10.44023056973261 | -0.19762191542962 | 37.22243610457459 |
| Na | 10.86789947984661 | 10.83949084717463 | 37.31106277073260 |
| Na | 5.21715297759380 | 5.27193795209444 | 5.51855138770084 |
| Na | 5.21715297759380 | 15.89219855912964 | 5.51855138770084 |
| Na | 15.83741358273927 | 5.27193795209444 | 5.51855138770084 |
| Na | 15.83741358273927 | 15.89219855912964 | 5.51855138770084 |
| Na | 5.21715297759380 | 5.27193795209444 | 16.13881199284631 |
| Na | 5.21715297759380 | 15.89219855912964 | 16.13881199284631 |
| Na | 15.83741358273927 | 5.27193795209444 | 16.13881199284631 |
| Na | 15.83741358273927 | 15.89219855912964 | 16.13881199284631 |
| Na | 5.21715297759380 | 5.27193795209444 | 26.75907259988151 |
| Na | 5.21715297759380 | 15.89219855912964 | 26.75907259988151 |
| Na | 15.83741358273927 | 5.27193795209444 | 26.75907259988151 |
| Na | 15.83741358273927 | 15.89219855912964 | 26.75907259988151 |
| Na | 5.32880966800696 | 5.35677063211884 | 36.80014219161080 |
| Na | 5.74563995188585 | 16.16384631543169 | 37.54555323908139 |
| Na | 15.87526972542862 | 5.11710276016293 | 36.76741707864944 |
| Na | 15.67653307567568 | 15.54147502226489 | 37.21687460468394 |
| Na | -0.09297732592380 | 5.27193795209444 | 0.20842108418324 |
| Na | -0.09297732592380 | 15.89219855912964 | 0.20842108418324 |
| Na | 10.52728328111139 | 5.27193795209444 | 0.20842108418324 |
| Na | 10.52728328111139 | 15.89219855912964 | 0.20842108418324 |
| Na | -0.09297732592380 | 5.27193795209444 | 10.82868169121844 |
| Na | -0.09297732592380 | 15.89219855912964 | 10.82868169121844 |
| Na | 10.52728328111139 | 5.27193795209444 | 10.82868169121844 |
| Na | 10.52728328111139 | 15.89219855912964 | 10.82868169121844 |
| Na | -0.09297732592380 | 5.27193795209444 | 21.44894229636391 |
| Na | -0.09297732592380 | 15.89219855912964 | 21.44894229636391 |
| Na | 10.52728328111139 | 5.27193795209444 | 21.44894229636391 |
| Na | 10.52728328111139 | 15.89219855912964 | 21.44894229636391 |
| Na | -0.05000227420980 | 5.26012794615985 | 31.92514206622747 |
| Na | -0.01193762858845 | 15.87911072416878 | 32.03612631271687 |
| Na | 10.56960373169570 | 5.27861251768025 | 31.98390308118688 |
| Na | 10.56288038471970 | 15.88913886009696 | 31.79269877772295 |
| Na | 5.21715297759380 | -0.03819235142316 | 0.20842108418324 |
| Na | 5.21715297759380 | 10.58206825561204 | 0.20842108418324 |
| Na | 15.83741358273927 | -0.03819235142316 | 0.20842108418324 |
| Na | 15.83741358273927 | 10.58206825561204 | 0.20842108418324 |
| Na | 5.21715297759380 | -0.03819235142316 | 10.82868169121844 |
| Na | 5.21715297759380 | 10.58206825561204 | 10.82868169121844 |
| Na | 15.83741358273927 | -0.03819235142316 | 10.82868169121844 |
| Na | 15.83741358273927 | 10.58206825561204 | 10.82868169121844 |
| Na | 5.21715297759380 | -0.03819235142316 | 21.44894229636391 |
| Na | 5.21715297759380 | 10.58206825561204 | 21.44894229636391 |
| Na | 15.83741358273927 | -0.03819235142316 | 21.44894229636391 |
| Na | 15.83741358273927 | 10.58206825561204 | 21.44894229636391 |
| Na | 5.24062303969497 | -0.03712795184490 | 31.94452710736424 |
| Na | 5.35865279178043 | 10.69157727228415 | 32.04102733065012 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 15.80248805567044 | -0.17700765469169 | 32.00199143761011 |
| Na | 15.91202032542252 | 10.50929811318322 | 31.89457494680154 |
| Cl | 5.21715297759380 | 5.27193795209444 | 0.20842108418324 |
| Cl | 5.21715297759380 | 15.89219855912964 | 0.20842108418324 |
| Cl | 15.83741358273927 | 5.27193795209444 | 0.20842108418324 |
| Cl | 15.83741358273927 | 15.89219855912964 | 0.20842108418324 |
| Cl | 5.21715297759380 | 5.27193795209444 | 10.82868169121844 |
| Cl | 5.21715297759380 | 15.89219855912964 | 10.82868169121844 |
| Cl | 15.83741358273927 | 5.27193795209444 | 10.82868169121844 |
| Cl | 15.83741358273927 | 15.89219855912964 | 10.82868169121844 |
| Cl | 5.21715297759380 | 5.27193795209444 | 21.44894229636391 |
| Cl | 5.21715297759380 | 15.89219855912964 | 21.44894229636391 |
| Cl | 15.83741358273927 | 5.27193795209444 | 21.44894229636391 |
| Cl | 15.83741358273927 | 15.89219855912964 | 21.44894229636391 |
| Cl | 5.237844485694258 | 5.34137208351603 | 31.82270945595301 |
| Cl | 5.20514540457229 | 15.93354288302243 | 31.99506067240490 |
| Cl | 15.89631826790679 | 5.14478103825404 | 31.79375801267971 |
| Cl | 15.98501443252250 | 15.81097624433074 | 31.91882728181914 |
| Cl | -0.09297732592380 | -0.03819235142316 | 0.20842108418324 |
| Cl | -0.09297732592380 | 10.58206825561204 | 0.20842108418324 |
| Cl | 10.52728328111139 | -0.03819235142316 | 0.20842108418324 |
| Cl | 10.52728328111139 | 10.58206825561204 | 0.20842108418324 |
| Cl | -0.09297732592380 | -0.03819235142316 | 10.82868169121844 |
| Cl | -0.09297732592380 | 10.58206825561204 | 10.82868169121844 |
| Cl | 10.52728328111139 | -0.03819235142316 | 10.82868169121844 |
| Cl | 10.52728328111139 | 10.58206825561204 | 10.82868169121844 |
| Cl | -0.09297732592380 | -0.03819235142316 | 21.44894229636391 |
| Cl | -0.09297732592380 | 10.58206825561204 | 21.44894229636391 |
| Cl | 10.52728328111139 | -0.03819235142316 | 21.44894229636391 |
| Cl | 10.52728328111139 | 10.58206825561204 | 21.44894229636391 |
| Cl | -0.11770676576536 | -0.03997113550681 | 31.81422417180177 |
| Cl | 0.04262595882748 | 10.55816052538141 | 31.81321425869687 |
| Cl | 10.53811161967748 | 0.03885791296438 | 31.91614625366629 |
| Cl | 10.60916259888189 | 10.51272041097504 | 31.93833311991900 |
| Cl | 5.21715297759380 | -0.03819235142316 | 5.51855138770084 |
| Cl | 5.21715297759380 | 10.58206825561204 | 5.51855138770084 |
| Cl | 15.83741358273927 | -0.03819235142316 | 5.51855138770084 |
| Cl | 15.83741358273927 | 10.58206825561204 | 5.51855138770084 |
| Cl | 5.21715297759380 | -0.03819235142316 | 16.13881199284631 |
| Cl | 5.21715297759380 | 10.58206825561204 | 16.13881199284631 |
| Cl | 15.83741358273927 | -0.03819235142316 | 16.13881199284631 |
| Cl | 15.83741358273927 | 10.58206825561204 | 16.13881199284631 |
| Cl | 5.21715297759380 | -0.03819235142316 | 26.75907259988151 |
| Cl | 5.21715297759380 | 10.58206825561204 | 26.75907259988151 |
| Cl | 15.83741358273927 | -0.03819235142316 | 26.75907259988151 |
| Cl | 15.83741358273927 | 10.58206825561204 | 26.75907259988151 |
| Cl | 5.00066757220982 | 0.21699849626253 | 37.04067552222715 |
| Cl | 5.23170231729110 | 10.55765429987787 | 37.35312994510382 |
| Cl | 15.98465751994927 | -0.06130314257290 | 37.28550338207421 |
| Cl | 16.22395064976596 | 10.19540097322725 | 36.93838130226601 |
| Cl | -0.09297732592380 | 5.27193795209444 | 5.51855138770084 |
| Cl | -0.09297732592380 | 15.89219855912964 | 5.51855138770084 |
| Cl | 10.52728328111139 | 5.27193795209444 | 5.51855138770084 |
| Cl | 10.52728328111139 | 15.89219855912964 | 5.51855138770084 |
| Cl | -0.09297732592380 | 5.27193795209444 | 16.13881199284631 |
| Cl | -0.09297732592380 | 15.89219855912964 | 16.13881199284631 |
| Cl | 10.52728328111139 | 5.27193795209444 | 16.13881199284631 |
| Cl | 10.52728328111139 | 15.89219855912964 | 16.13881199284631 |
| Cl | -0.09297732592380 | 5.27193795209444 | 26.75907259988151 |
| Cl | -0.09297732592380 | 15.89219855912964 | 26.75907259988151 |
| Cl | 10.52728328111139 | 5.27193795209444 | 26.75907259988151 |
| Cl | 10.52728328111139 | 15.89219855912964 | 26.75907259988151 |
| Cl | -0.01247052001734 | 5.22854028014012 | 37.22857412022173 |
| Cl | 0.01303804256720 | 15.87410062557441 | 37.41070603942190 |
| Cl | 10.60596596273529 | 5.27275411724892 | 37.26428570532841 |
| Cl | 10.66627486559177 | 15.94084863603125 | 36.59561710853630 |
| N | 10.42814441622965 | -6.05149783407868 | 45.89896561169145 |
| C | 8.11500069798546 | -7.44595466808413 | 45.93038291701129 |
| C | 12.67447068036135 | -7.41947745645437 | 45.18439014569899 |
| C | 10.25983358919054 | -3.50867732038774 | 44.93075538543203 |
| C | 6.72307686988549 | -7.23122681004161 | 48.36049770607393 |

| | | | |
|---|-------------------|-------------------|-------------------|
| C | 12.98576002283128 | -7.95542102547399 | 42.35988140553539 |
| C | 8.95369420923672 | -2.92579992184350 | 42.40130176066909 |
| O | 7.23228098242208 | -5.83683497694568 | 50.12339073691644 |
| O | 4.67340984178301 | -8.73473877684984 | 48.42054855737941 |
| O | 11.58047973142233 | -9.65217895774131 | 41.44843120481560 |
| O | 14.61598281851029 | -6.65053646902060 | 41.21920522054348 |
| O | 7.13754215773950 | -4.30163074210754 | 41.68545588093568 |
| O | 9.72963613118617 | -0.94273253046142 | 41.34865987505598 |
| H | 8.43346776640896 | -9.45468581013958 | 45.46073003716735 |
| H | 6.88284180736681 | -6.75206709222861 | 44.35613076858524 |
| H | 12.67420750387310 | -9.24187498665428 | 46.21646661054589 |
| H | 14.33965059555055 | -6.32001931818641 | 45.82627736243399 |
| H | 12.20219906907601 | -2.75889529103660 | 44.78247521501166 |
| H | 9.26584480572647 | -2.30277972696099 | 46.34444530013763 |
| H | 3.82415950214612 | -8.42724930701041 | 50.06756115393925 |

NTA adsorbed (110) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | -0.17726733140716 | 7.48982612461360 | 4.11318466777784 |
| Na | -0.17726733140716 | 22.50914271042150 | 4.11318466777784 |
| Na | 10.44299327373831 | 7.48982612461360 | 4.11318466777784 |
| Na | 10.44299327373831 | 22.50914271042150 | 4.11318466777784 |
| Na | -0.17726733140716 | -0.01983216734548 | 11.62284296162665 |
| Na | -0.17726733140716 | 14.99948441846241 | 11.62284296162665 |
| Na | 10.44299327373831 | -0.01983216734548 | 11.62284296162665 |
| Na | 10.44299327373831 | 14.99948441846241 | 11.62284296162665 |
| Na | -0.17726733140716 | 7.48982612461360 | 19.13250125358573 |
| Na | -0.17726733140716 | 22.50914271042150 | 19.13250125358573 |
| Na | 10.44299327373831 | 7.48982612461360 | 19.13250125358573 |
| Na | 10.44299327373831 | 22.50914271042150 | 19.13250125358573 |
| Na | -0.19644502990377 | -0.12050406120777 | 26.03490902068907 |
| Na | -0.28640375833811 | 15.36454848028765 | 26.30166779283383 |
| Na | 10.43652428011928 | -0.11223906998982 | 26.04010434078958 |
| Na | 10.35394712995452 | 15.40679750300388 | 26.28038266798318 |
| Na | 5.13286297211044 | 11.24465527153801 | 0.35835552274316 |
| Na | 5.13286297211044 | 26.26397185734590 | 0.35835552274316 |
| Na | 15.75312357725591 | 11.24465527153801 | 0.35835552274316 |
| Na | 15.75312357725591 | 26.26397185734590 | 0.35835552274316 |
| Na | 5.13286297211044 | 3.73499697957892 | 7.86801381470224 |
| Na | 5.13286297211044 | 18.75431356538682 | 7.86801381470224 |
| Na | 15.75312357725591 | 3.73499697957892 | 7.86801381470224 |
| Na | 15.75312357725591 | 18.75431356538682 | 7.86801381470224 |
| Na | 5.13286297211044 | 11.24465527153801 | 15.37767210666132 |
| Na | 5.13286297211044 | 26.26397185734590 | 15.37767210666132 |
| Na | 15.75312357725591 | 11.24465527153801 | 15.37767210666132 |
| Na | 15.75312357725591 | 26.26397185734590 | 15.37767210666132 |
| Na | 5.12638912000554 | 3.72696616511211 | 22.82339902117342 |
| Na | 5.04128775683097 | 18.78429905167791 | 22.93407045373844 |
| Na | 15.74486649454179 | 3.70619783311349 | 22.82154302288031 |
| Na | 15.65137701504360 | 18.71383369104072 | 22.89209843085707 |
| Na | 5.13286297211044 | 3.73499697957892 | 0.35835552274316 |
| Na | 5.13286297211044 | 18.75431356538682 | 0.35835552274316 |
| Na | 15.75312357725591 | 3.73499697957892 | 0.35835552274316 |
| Na | 15.75312357725591 | 18.75431356538682 | 0.35835552274316 |
| Na | 5.13286297211044 | 11.24465527153801 | 7.86801381470224 |
| Na | 5.13286297211044 | 26.26397185734590 | 7.86801381470224 |
| Na | 15.75312357725591 | 11.24465527153801 | 7.86801381470224 |
| Na | 15.75312357725591 | 26.26397185734590 | 7.86801381470224 |
| Na | 5.13286297211044 | 3.73499697957892 | 15.37767210666132 |
| Na | 5.13286297211044 | 18.75431356538682 | 15.37767210666132 |
| Na | 15.75312357725591 | 3.73499697957892 | 15.37767210666132 |
| Na | 15.75312357725591 | 18.75431356538682 | 15.37767210666132 |
| Na | 5.09607803579284 | 11.31573107985398 | 22.84231116023714 |
| Na | 5.07119487806938 | 26.19731322904505 | 22.85137692856973 |
| Na | 15.71581251094950 | 11.28270953122458 | 22.84477810320701 |
| Na | 15.70541594456735 | 26.13660304473565 | 22.85995858308417 |
| Na | -0.17726733140716 | -0.01983216734548 | 4.11318466777784 |
| Na | -0.17726733140716 | 14.99948441846241 | 4.11318466777784 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Na | 10.44299327373831 | -0.01983216734548 | 4.11318466777784 |
| Na | 10.44299327373831 | 14.99948441846241 | 4.11318466777784 |
| Na | -0.17726733140716 | 7.48982612461360 | 11.62284296162665 |
| Na | -0.17726733140716 | 22.50914271042150 | 11.62284296162665 |
| Na | 10.44299327373831 | 7.48982612461360 | 11.62284296162665 |
| Na | 10.44299327373831 | 22.50914271042150 | 11.62284296162665 |
| Na | -0.17726733140716 | -0.01983216734548 | 19.13250125358573 |
| Na | -0.17726733140716 | 14.99948441846241 | 19.13250125358573 |
| Na | 10.44299327373831 | -0.01983216734548 | 19.13250125358573 |
| Na | 10.44299327373831 | 14.99948441846241 | 19.13250125358573 |
| Na | -0.19906544887061 | 7.54870069132614 | 26.04709213226005 |
| Na | -0.33505318895339 | 22.05893185829536 | 26.55497591960927 |
| Na | 10.42600835296590 | 7.55339226146433 | 26.04780684557779 |
| Na | 10.23243311217816 | 22.12049076963009 | 26.48042833669209 |
| Cl | 5.13286297211044 | -0.01983216734548 | 4.11318466777784 |
| Cl | 5.13286297211044 | 14.99948441846241 | 4.11318466777784 |
| Cl | 15.75312357725591 | -0.01983216734548 | 4.11318466777784 |
| Cl | 15.75312357725591 | 14.99948441846241 | 4.11318466777784 |
| Cl | 5.13286297211044 | 7.48982612461360 | 11.62284296162665 |
| Cl | 5.13286297211044 | 22.50914271042150 | 11.62284296162665 |
| Cl | 15.75312357725591 | 7.48982612461360 | 11.62284296162665 |
| Cl | 15.75312357725591 | 22.50914271042150 | 11.62284296162665 |
| Cl | 5.13286297211044 | -0.01983216734548 | 19.13250125358573 |
| Cl | 5.13286297211044 | 14.99948441846241 | 19.13250125358573 |
| Cl | 15.75312357725591 | -0.01983216734548 | 19.13250125358573 |
| Cl | 15.75312357725591 | 14.99948441846241 | 19.13250125358573 |
| Cl | 5.11046888604977 | 7.46398001914863 | 26.38620165613527 |
| Cl | 4.92506890850410 | 22.63942403129655 | 26.35897326892218 |
| Cl | 15.73220478148376 | 7.42581058821364 | 26.38723561600510 |
| Cl | 15.57640556466685 | 22.44560509142772 | 26.18736005099334 |
| Cl | -0.17726733140716 | 3.73499697957892 | 0.35835552274316 |
| Cl | -0.17726733140716 | 18.75431356538682 | 0.35835552274316 |
| Cl | 10.44299327373831 | 3.73499697957892 | 0.35835552274316 |
| Cl | 10.44299327373831 | 18.75431356538682 | 0.35835552274316 |
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| Cl | -0.17726733140716 | 26.26397185734590 | 7.86801381470224 |
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NTA adsorbed (111) surface of NaCl:

| | | | |
|----|-------------------|-------------------|-------------------|
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| Na | 0.00021954838120 | 15.00421962426656 | 3.29706134427511 |
| Na | 13.00732925855620 | 7.49456133230747 | 3.29706134427511 |
| Na | 13.00732925855620 | 22.51387791811536 | 3.29706134427511 |
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| Na | 8.67162602120129 | 15.00421962426656 | 9.42867166455839 |
| Na | 21.67873573137628 | 7.49456133230747 | 9.42867166455839 |
| Na | 21.67873573137628 | 22.51387791811536 | 9.42867166455839 |
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| Na | 12.77244869971260 | 7.93652669140982 | 21.61419722838903 |
| Na | 12.86271634356632 | 22.61414541436636 | 21.08391083420405 |
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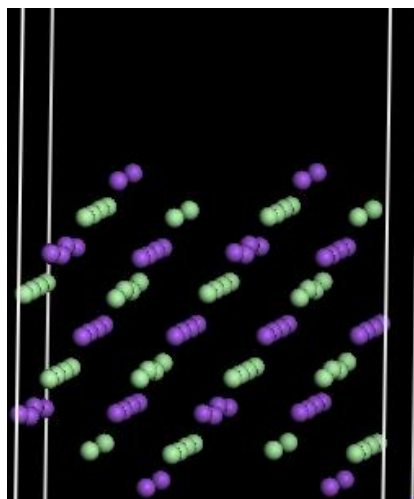


Figure S1. LDA/PWC/DND level optimized geometry of Na^+ terminated octopolar reconstructed (111) NaCl surface (purple: sodium, green: chloride).

Table S1. Computed Surface Energies for completely relaxed (100), (110) and (111) NaCl Surfaces in Presence of Formamide.

| Method ^a | (100) | (110) | (111) |
|-----------------------------|-------|-------|-------|
| GGA/BLYP/DND//LDA/PWC/DND | 153 | 382 | 574 |
| GGA/VWN-BP/DNP//LDA/PWC/DND | 84 | 291 | 454 |

^a GGA/BLYP/DNP and GGA/VWN-BP/DNP single point calculations were performed in implicit aqueous phase with LDA/PWC/DND optimized geometries in implicit aqueous phase.

The above tabulated values are surface energies computed with equation 4 in the main manuscript which does not involve the bulk energy term. Some of the recent studies in the literature (*Nature*, **2008**, 453, 638 and references therein) suggested equation (A) for calculating surface energies of ionic solids in presence of additives which involves bulk energy term (E_{bulk}). Therefore, we have verified our results with this equation. The computed surface energies for (100), (110) and (111) NaCl crystal surfaces in presence of additives are presented in Table A and the corresponding decreased surface energies values are given in Table B. The plots of interaction energies versus decreased surfaces energies calculated from equation A are depicted in Figure S2. From these results, it has been observed that the relative trends of stability of (100), (110) and (111) NaCl surfaces computed from equation 4 were well reproduced with equation A.

$$\gamma_{additive} = \frac{(E_{slab}'' - N \times E_{bulk} - m \times E_{additive})}{2 \times A} \dots\dots\dots (A)$$

Table A. Computed Surface Energies for (100), (110) and (111) NaCl Crystal Surfaces in Presence of Additives.

| Additive | Surface Energies (erg/cm ²) | | |
|-------------|---|----------|---------|
| | (100) | (110) | (111) |
| Formamide | 58.7 | 277.3 | 428.45 |
| | (83.6) | (291.18) | (454.1) |
| Citric acid | 1.68 | 217.77 | 313.5 |
| | (42.46) | (241.5) | (351.9) |
| NTA | -93.8 | 150.3 | 164.8 |

^a GGA/BLYP/DNP and GGA/VWN-BP/DNP () single point calculations were performed in implicit aqueous phase with LDA/PWC/DND optimized geometries in implicit aqueous phase.

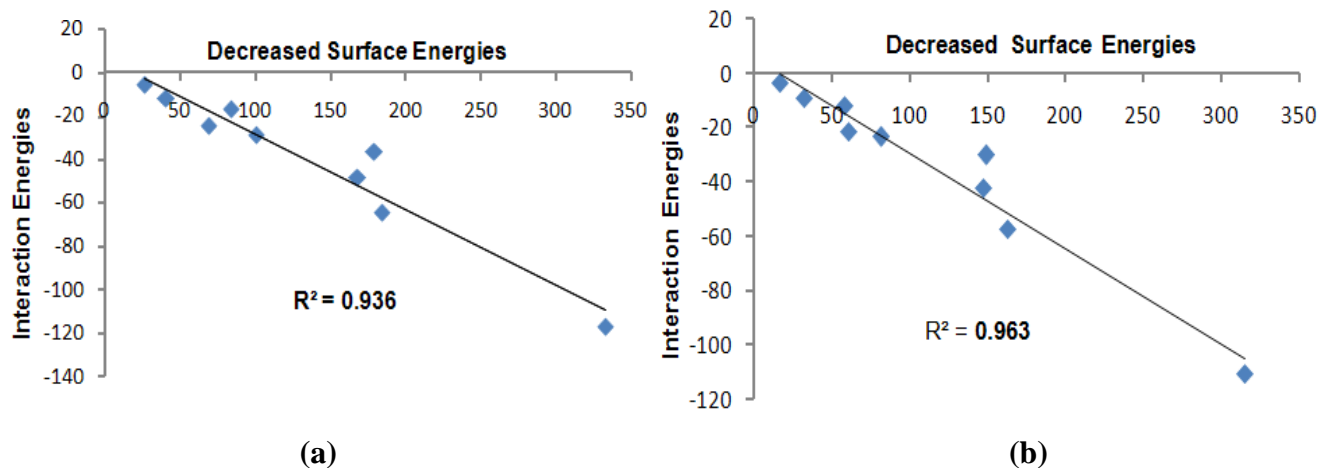


Figure S2. Plots of linear fits computed at GGA/BLYP/DNP//LDA/PWC/DND **(a)** and GGA/VWN-BP/DNP//LDA/PWC/DND **(b)** for decreased surface energies (erg/cm^2) versus interaction energies (kcal/mol).

Table B. Computed Decrease in Surface Energies for (100), (110) and (111) NaCl Crystal Surfaces in Presence of Additives and their Corresponding Interaction Energies.

| Additive | Decrease in Surface Energies (erg/cm^2) | | | Interaction Energies (kcal/mol) | | |
|-------------|---|---------|---------|---------------------------------|---------|----------|
| | (100) | (110) | (111) | (100) | (110) | (111) |
| Formamide | 26.5 | 40.8 | 69.1 | -5.4 | -11.7 | -24.3 |
| | (17.1) | (32.3) | (61.0) | (-3.5) | (-9.3) | (-21.4) |
| Citric acid | 83.4 | 100.4 | 184.1 | -16.9 | -28.8 | -64.6 |
| | (58.2) | (82.0) | (163.2) | (-11.8) | (-23.5) | (-57.3) |
| NTA | 179.1 | 167.9 | 332.7 | -36.3 | -48.1 | -116.8 |
| | (149.1) | (147.7) | (315.1) | (-30.2) | (-42.4) | (-110.6) |

Table S2. The surface energy values of clean (100), (110) and (111) NaCl surfaces and the corresponding decreased surface energy values of adsorbed surfaces.

| Entry | (100) | (110) | (111) |
|-------------|-------|-------|-------|
| NaCl | 38 | 271 | 461 |
| Formamide | -127 | 89 | 422 |
| Citric acid | -167 | 45 | 331 |

| | | | |
|-----|------|------|-----|
| NTA | -215 | -7.1 | 184 |
|-----|------|------|-----|
